CALIFORNIA INSTITUTE OF TECHNOLOGY

PASADENA, CALIFORNIA 91125

ENVIRONMENTAL QUALITY LABORATORY 105-96

Conference

on

PHOTOCHEMICAL MODELING AS A TOOL FOR DECISION MAKERS

February 1 – 3, 1988

GRAPHICS PACKAGE

Sponsored by

Environmental Quality Laboratory

Caltech

and

California Air Resources Board

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HISTORICAL PERIODS

1. Period of development 1969 - 1975

2. Period of expanding application 1976 - 1982

3. Period of acceptance
and widespread use 1983 -

THE PERIOD OF DEVELOPMENT

1. The situation in 1969

2. Model development in California

3. Progress during the period

4. Situation at the end of 1975

PIONEERING EFFORTS IN CALIFORNIA

1. System Development Corp. (now Pacific Environmental Services)

   Simple trajectory model

2. General Research Corp. (now ERT)

   Trajectory model with vertical layers

3. Systems Science and Software
   (later, Xonics, then Form and Substance)

   Particle-in-cell approach

4. Caltech and Systems Applications, Inc. (joint)

   Three dimensional grid-based model

5. Lawrence Livermore Lab, BAAQMD, NASA

   Two dimensional grid-based model

PERIOD OF EXPANDING APPLICATION

1. Emergence of EKMA
2. Limited, varied use of models from area to area
3. Support of model development at Caltech by ARB
4. Variants of grid-based models
5. Early uses of models in regulatory arena
   a. SCAG / SCAQMD in 1978 - 1979
   b. Rule 1135 - the first two day simulations
   c. The SIPs
6. Performance evaluation, diagnostic assessment, data availability
7. Status of modeling in 1982

PERIOD OF ACCEPTANCE AND WIDESPREAD USE

1. Use of models in permitting
2. Use of models in long range planning
3. Large scale field studies
4. Continuing development
5. Performance evaluations
6. Status in 1988

BARRIERS TO PROGRESS – A RETROSPECTIVE EXAMINATION

1. Fragmented and sporadic support for model development

2. Difficulty in sustaining R & D efforts

3. Lack of suitable data bases

4. The adversary environment of the early 1980s

LESSONS FOR THE FUTURE

1. Plan modeling and monitoring in an integrated fashion.

2. Avoid contentiousness.

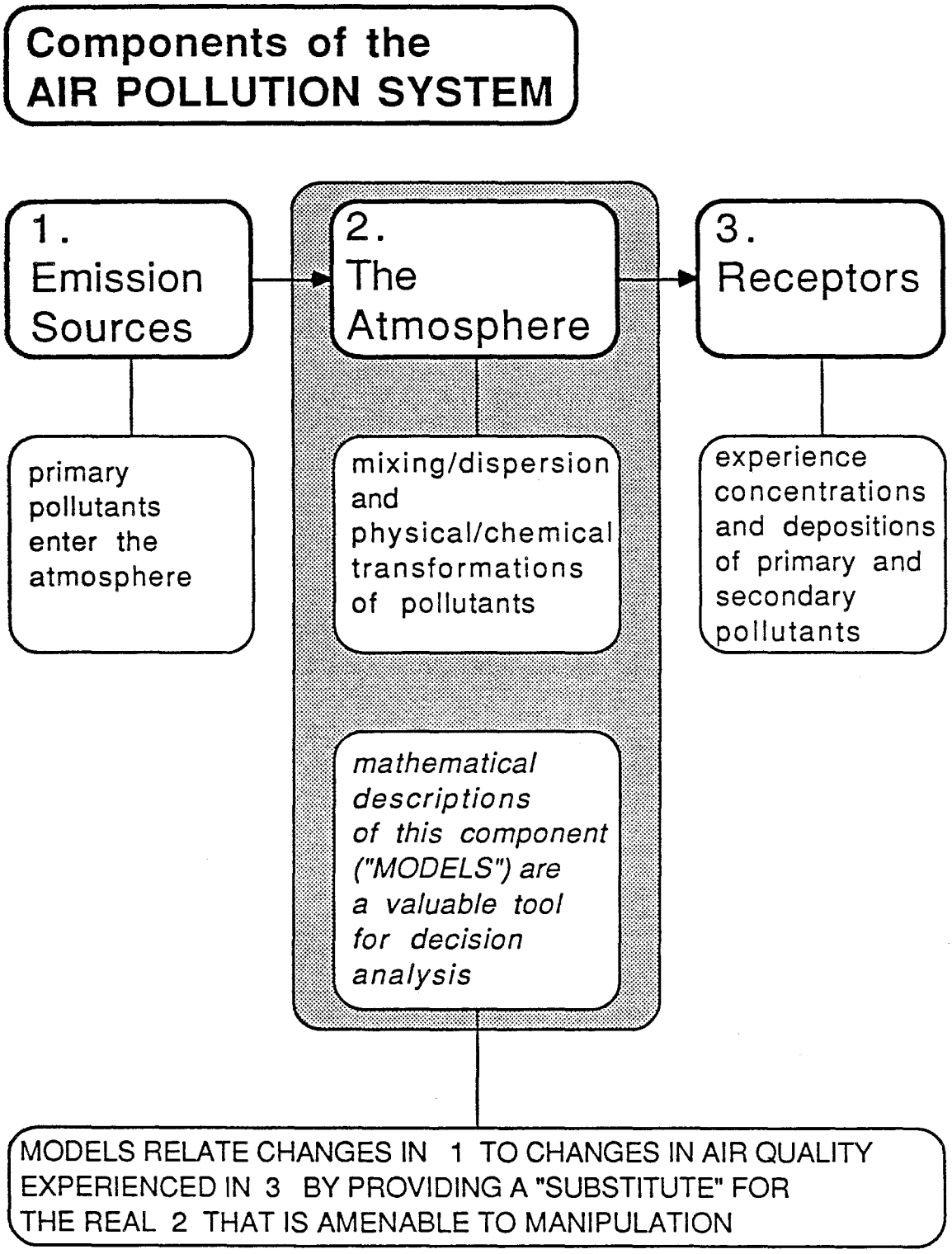
3. To the extent feasible, fund efforts at the levels needed.

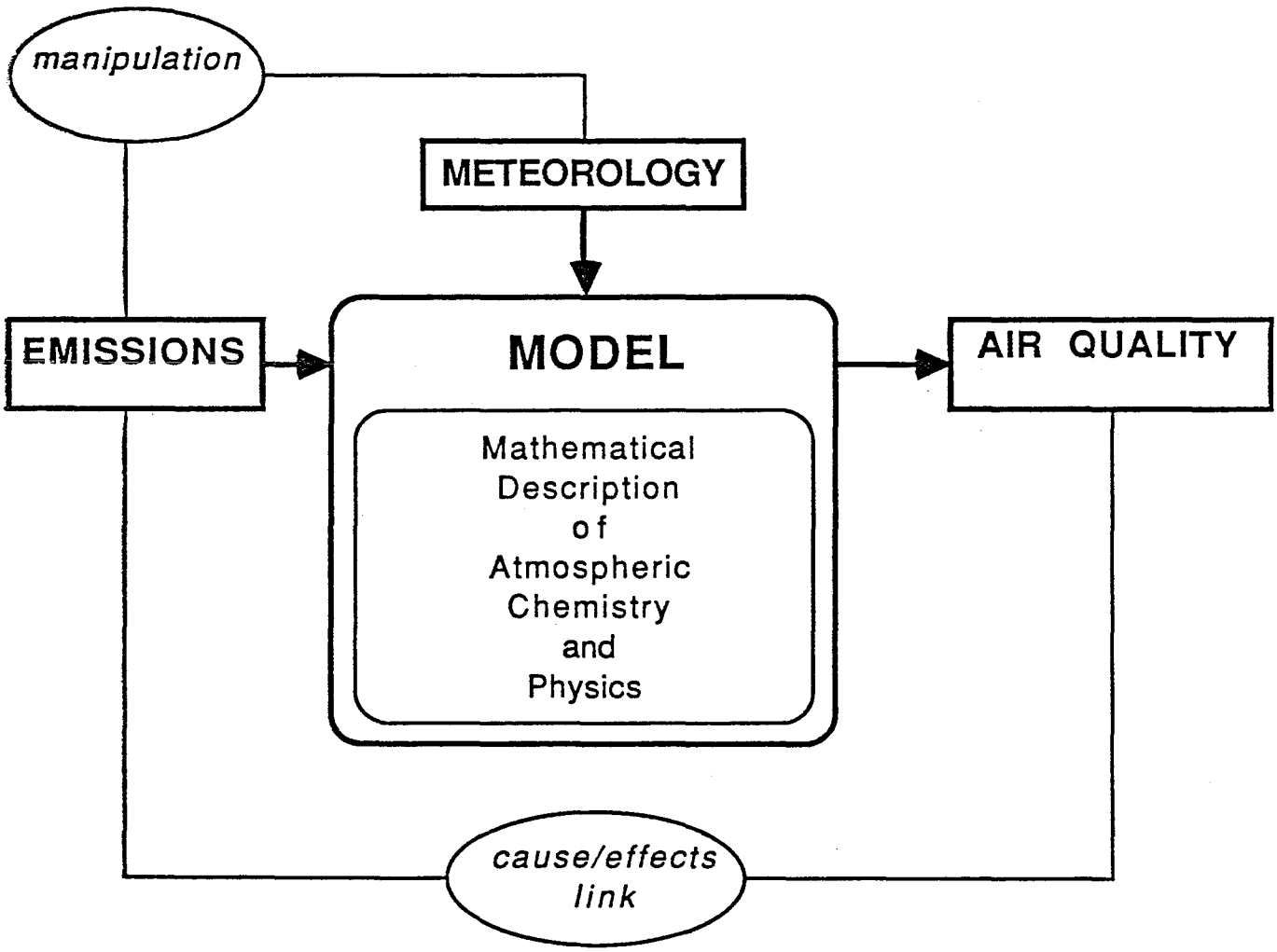
4. Develop expectations of models consistent with their capabilities.

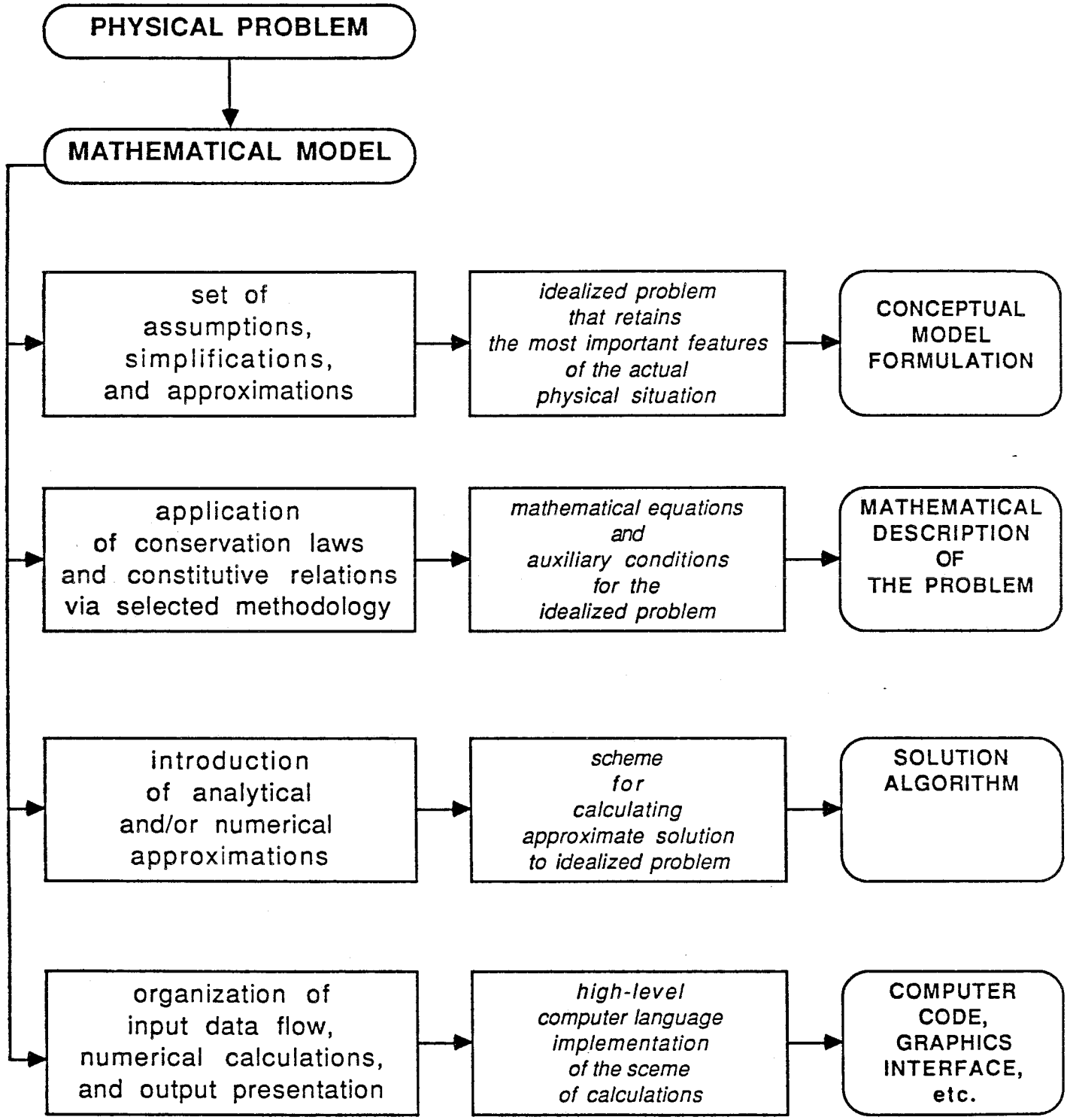
State-of-Art for Ozone Modeling

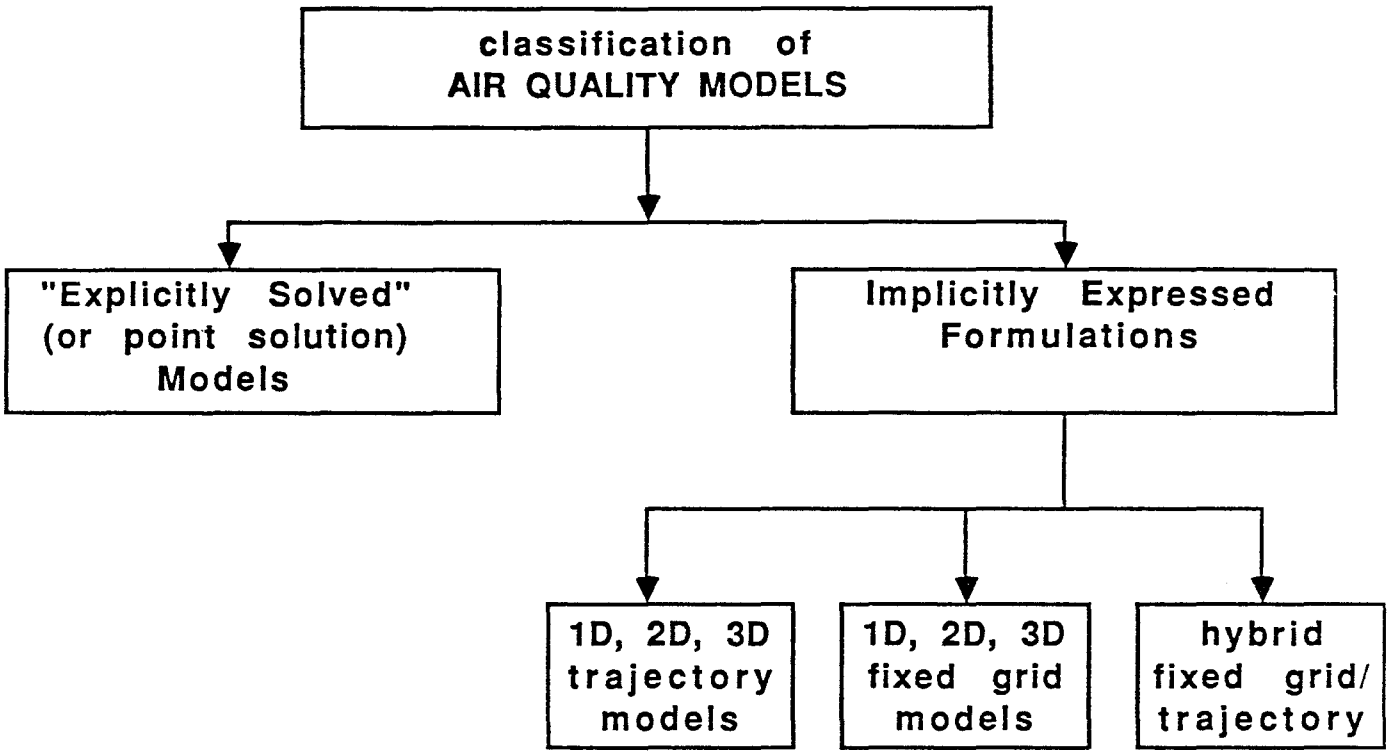
J. H. Seinfeld

California Institute of Technology
Pasadena, California 91125


Components of the
AIR POLLUTION SYSTEM
1.
Emission
Sources
2.
The
Atmosphere
3.
Receptors
primary
pollutants
enter the
atmosphere
mixing/dispersion
and
physical/chemical
transformations
of pollutants
experience
concentrations
and depositions
of primary and
secondary
pollutants
mathematical
descriptions
of this component
("MODELS") are
a valuable tool
for decision
analysis
MODELS RELATE CHANGES IN 1 TO CHANGES IN AIR QUALITY
EXPERIENCED IN 3 BY PROVIDING A "SUBSTITUTE" FOR
THE REAL 2 THAT IS AMENABLE TO MANIPULATION


manipulation
METEOROLOGY
EMISSIONS
MODEL
Mathematical
Description
of
Atmospheric
Chemistry
and
Physics
AIR QUALITY
cause/effects
link


PHYSICAL PROBLEM
MATHEMATICAL MODEL
set of assumptions, simplifications, and approximations
idealized problem that retains the most important features of the actual physical situation
CONCEPTUAL MODEL FORMULATION
application of conservation laws and constitutive relations via selected methodology
mathematical equations and auxiliary conditions for the idealized problem
MATHEMATICAL DESCRIPTION OF THE PROBLEM
introduction of analytical and/or numerical approximations
scheme for calculating approximate solution to idealized problem
SOLUTION ALGORITHM
organization of input data flow, numerical calculations, and output presentation
high-level computer language implementation of the sceme of calculations
COMPUTER CODE, GRAPHICS INTERFACE, etc.



mean concentrations
at any point
are given explicitly
(either through an
analytical formula
or an integral)
without
requiring calculations
of the
concentration field
at other points

explicit solution for
the mean concentration
is possible only after
the numerical
approximation of the
problem;
calculations in a cell or
grid of cells
are required
for an entire domain
such as a
trajectory
or a fixed grid

AIR QUALITY MODELS:

Conservation ("Balance") Laws

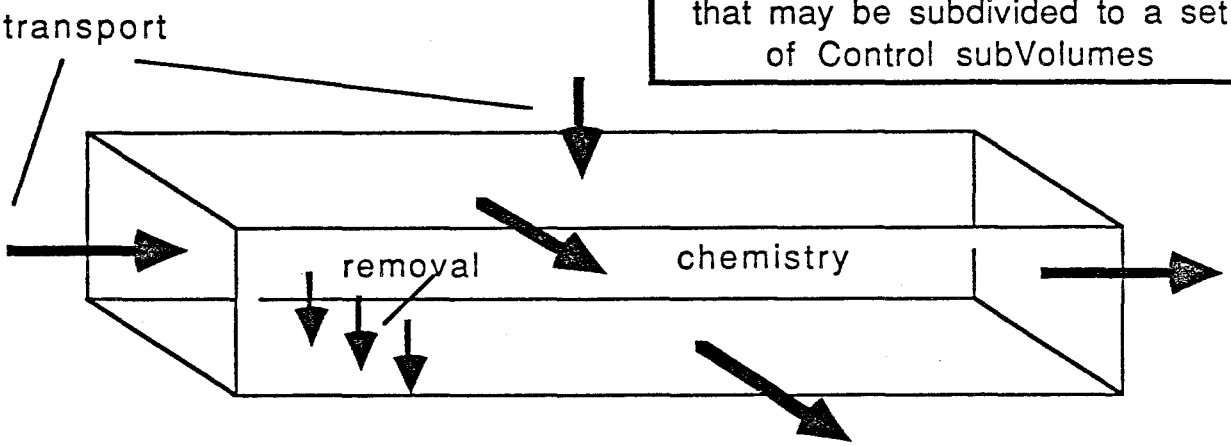
"Constitutive" Relations

differential eqns

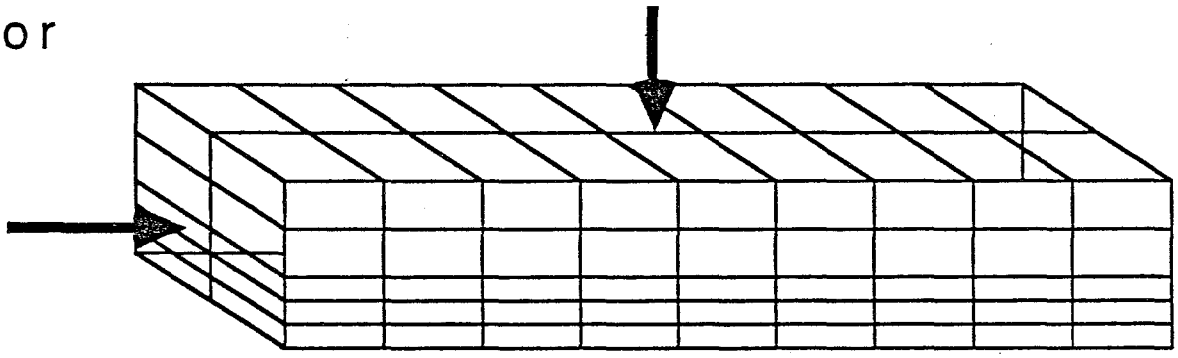
analytical or integral solns.

discretization

Applied to a Control Volume (CV) that may be subdivided to a set of Control subVolumes

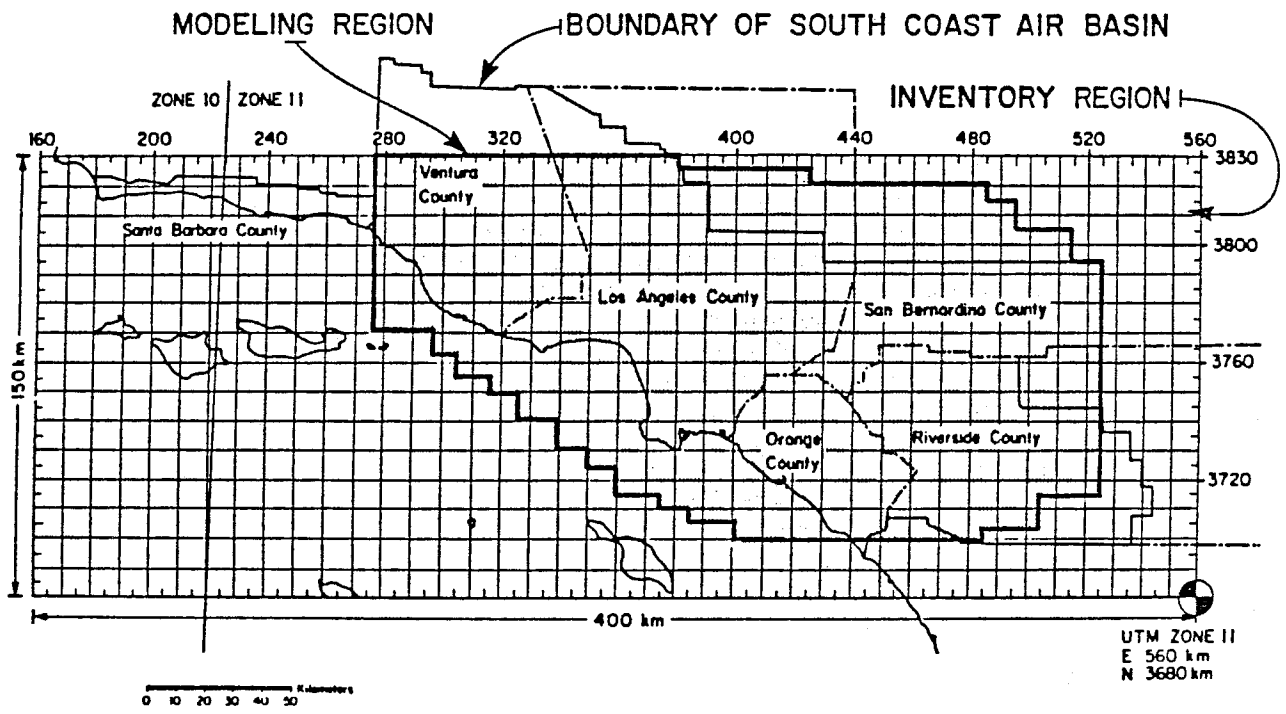


or

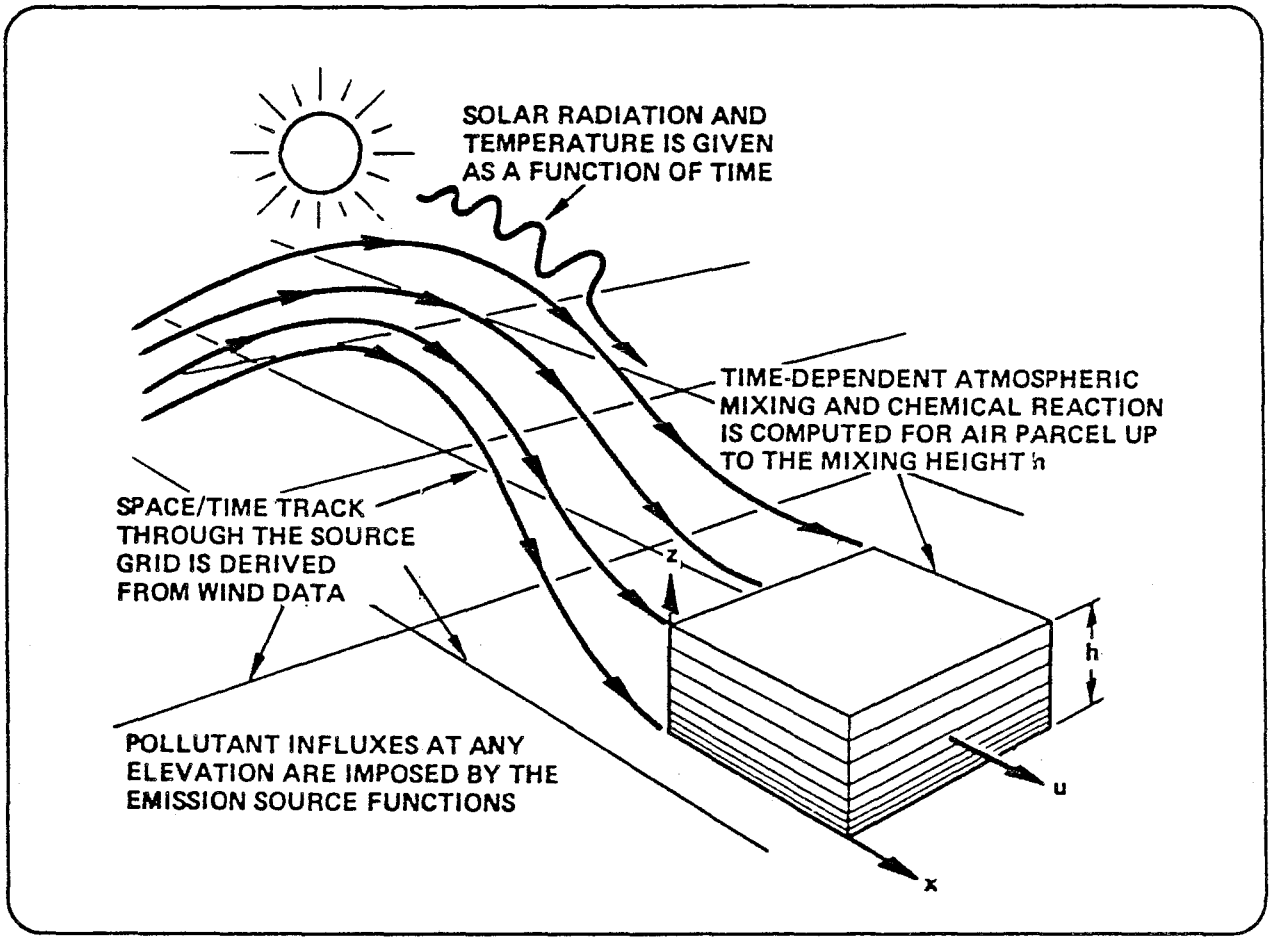


rate of accumulation of pollutant mass within the control (sub)volume	+	net outflow rate of pollutant mass by advection across the control surface	=	

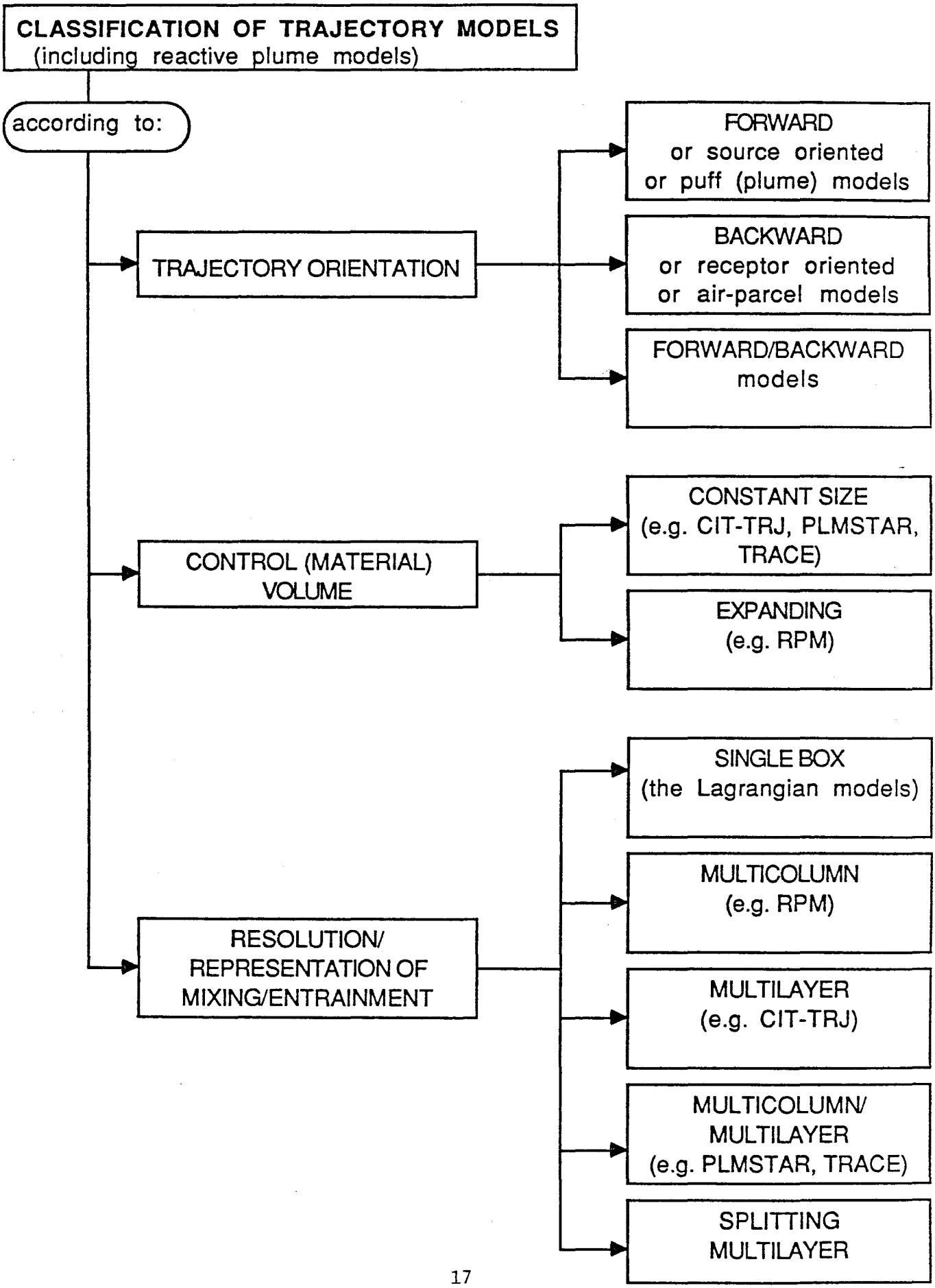
net inflow rate of pollutant mass by turbulent dispersion across control surface	+	net production of pollutant within the control (sub)volume by chemical reaction	-	net removal rate of pollutant (deposition or physical transf.)

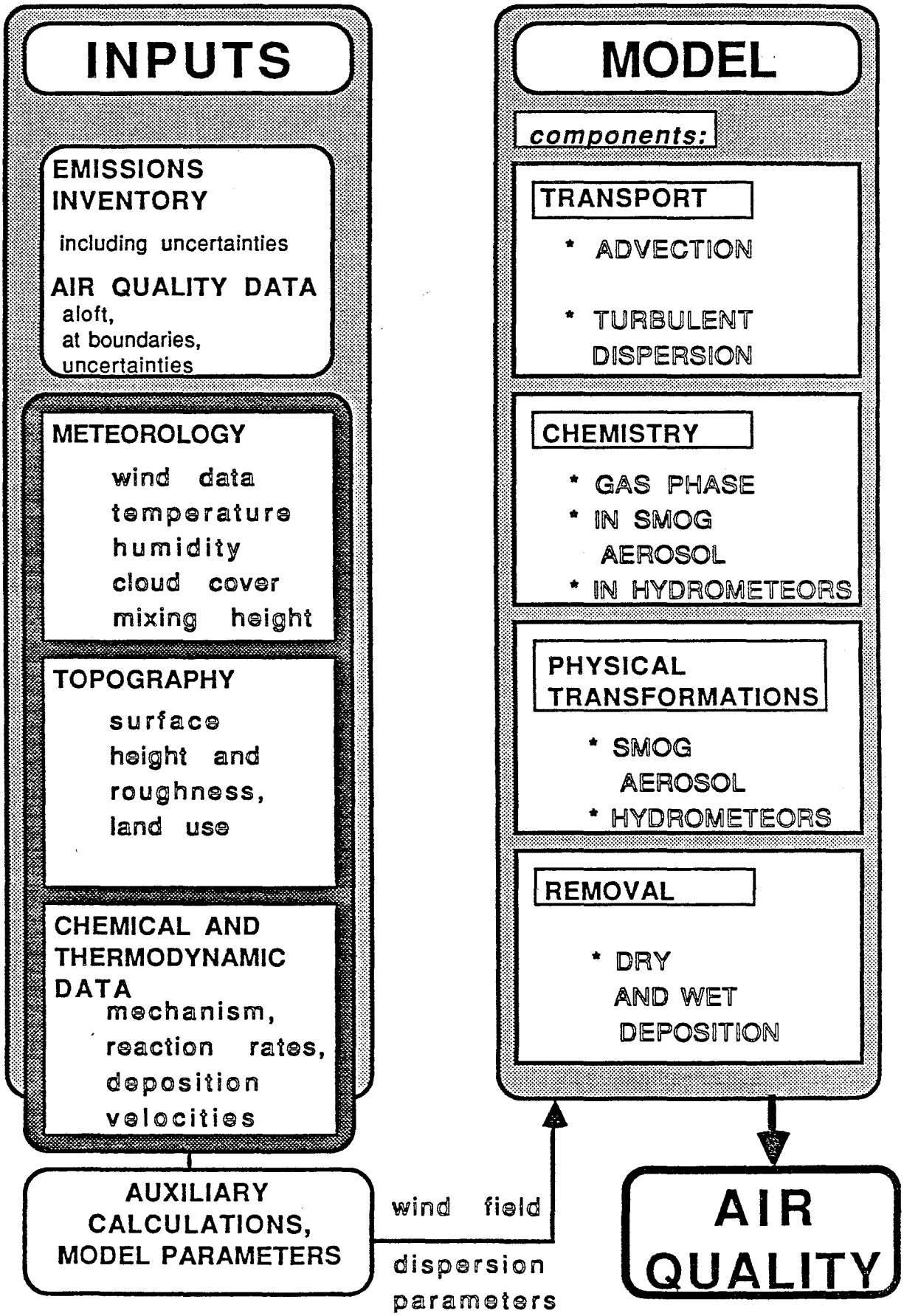


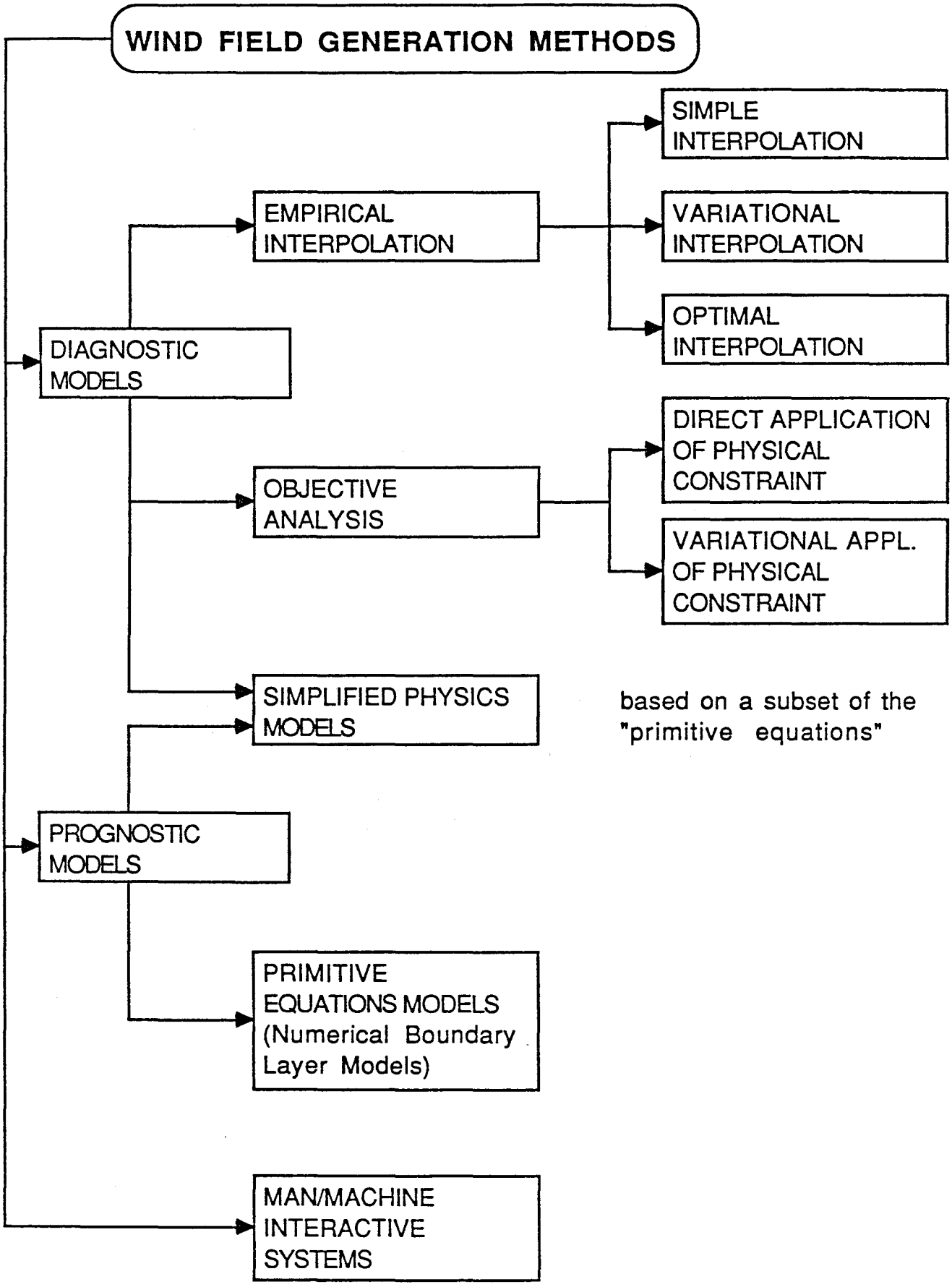
Airshed of the Caltech Grid Model



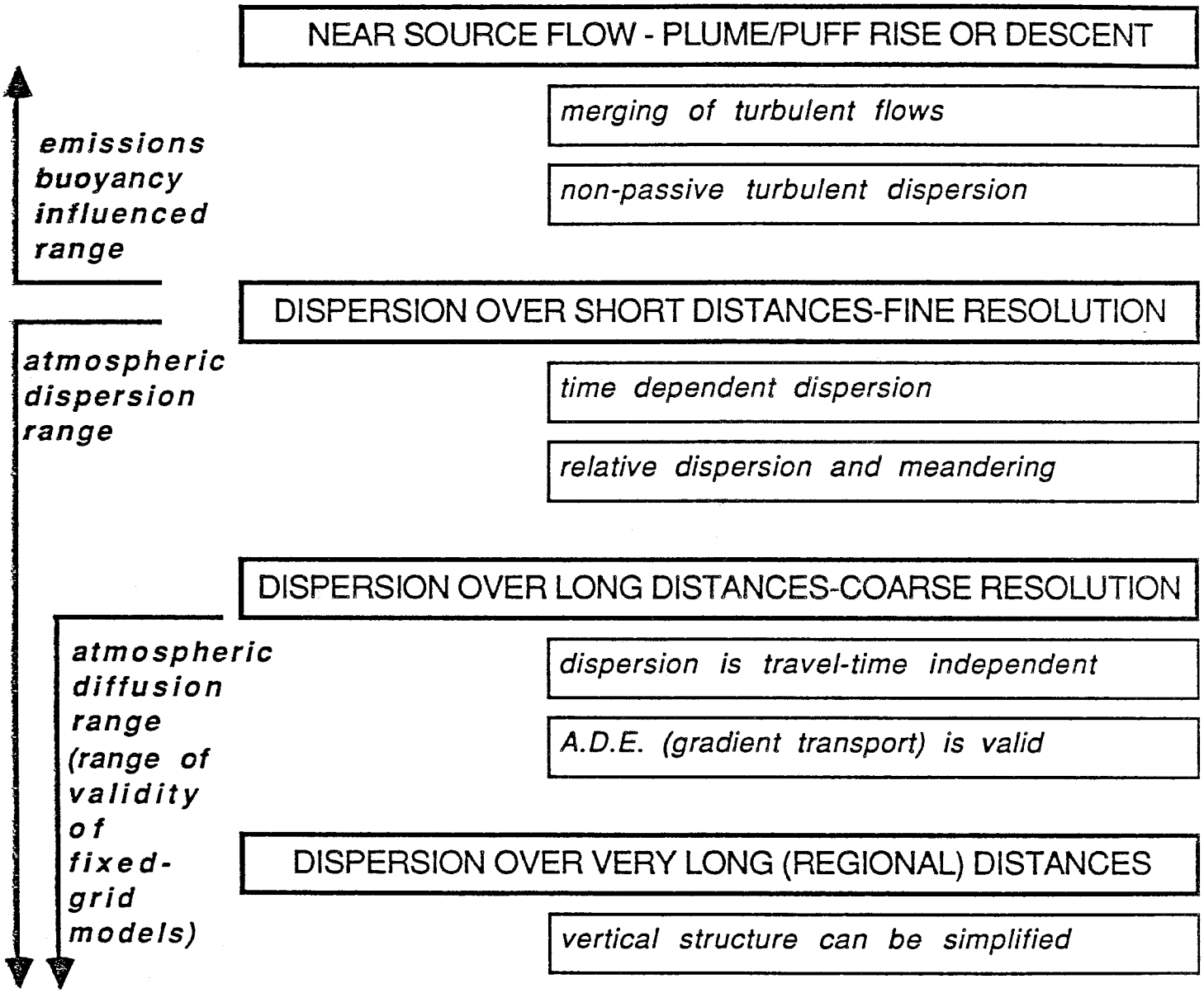
The Modeling Concept of a Trajectory Model


CLASSIFICATION OF TRAJECTORY MODELS
(including reactive plume models)
according to:
TRAJECTORY ORIENTATION
FORWARD
or source oriented
or puff (plume) models
BACKWARD
or receptor oriented
or air-parcel models
FORWARD/BACKWARD
models
CONTROL (MATERIAL)
VOLUME
CONSTANT SIZE
(e.g. CIT-TRJ, PLMSTAR,
TRACE)
EXPANDING
(e.g. RPM)
RESOLUTION/
REPRESENTATION OF
MIXING/ENTRAINMENT
SINGLE BOX
(the Lagrangian models)
MULTICOLUMN
(e.g. RPM)
MULTILAYER
(e.g. CIT-TRJ)
MULTICOLUMN/
MULTILAYER
(e.g. PLMSTAR, TRACE)
SPLITTING
MULTILAYER


INPUTS
EMISSIONS INVENTORY
including uncertainties
AIR QUALITY DATA
aloft,
at boundaries,
uncertainties
METEOROLOGY
wind data
temperature
humidity
cloud cover
mixing height
TOPOGRAPHY
surface
height and
roughness,
land use
CHEMICAL AND THERMODYNAMIC DATA
mechanism,
reaction rates,
deposition
velocities
AUXILIARY CALCULATIONS, MODEL PARAMETERS
wind field
dispersion parameters
MODEL
components:
TRANSPORT
* ADVECTION
* TURBULENT DISPERSION
CHEMISTRY
* GAS PHASE
* IN SMOG AEROSOL
* IN HYDROMETEORS
PHYSICAL TRANSFORMATIONS
* SMOG AEROSOL
* HYDROMETEORS
REMOVAL
* DRY AND WET DEPOSITION
AIR QUALITY


WIND FIELD GENERATION METHODS
DIAGNOSTIC MODELS
EMPIRICAL INTERPOLATION
SIMPLE INTERPOLATION
VARIATIONAL INTERPOLATION
OPTIMAL INTERPOLATION
OBJECTIVE ANALYSIS
DIRECT APPLICATION OF PHYSICAL CONSTRAINT
VARIATIONAL APPL. OF PHYSICAL CONSTRAINT
SIMPLIFIED PHYSICS MODELS
based on a subset of the "primitive equations"
PROGNOSTIC MODELS
PRIMITIVE EQUATIONS MODELS (Numerical Boundary Layer Models)
MAN/MACHINE INTERACTIVE SYSTEMS

TURBULENT DISPERSION



a local-scale ("subgrid") model must:

- discriminate between absolute and relative dispersion
- represent instantaneous gradients
- account for effects of incomplete fine-scale mixing (fluctuations)

an urban-scale model must:

- represent concentration gradients
- account for effects of vertical wind shear
- account for diurnal variations in reactivity of ambient air

both near-field and far-field models must incorporate adequate treatments of chemistry

both must account for special problems relevant to particular applications (complex terrain, overwater dispersion, etc.)

the local scale

must by necessity be treated through a trajectory type formulation

the urban scale

is better treated by fixed grid models that account for wind shear and vertical wind velocities; trajectory models are used as substitutes for computational efficiency

Model Performance Evaluation

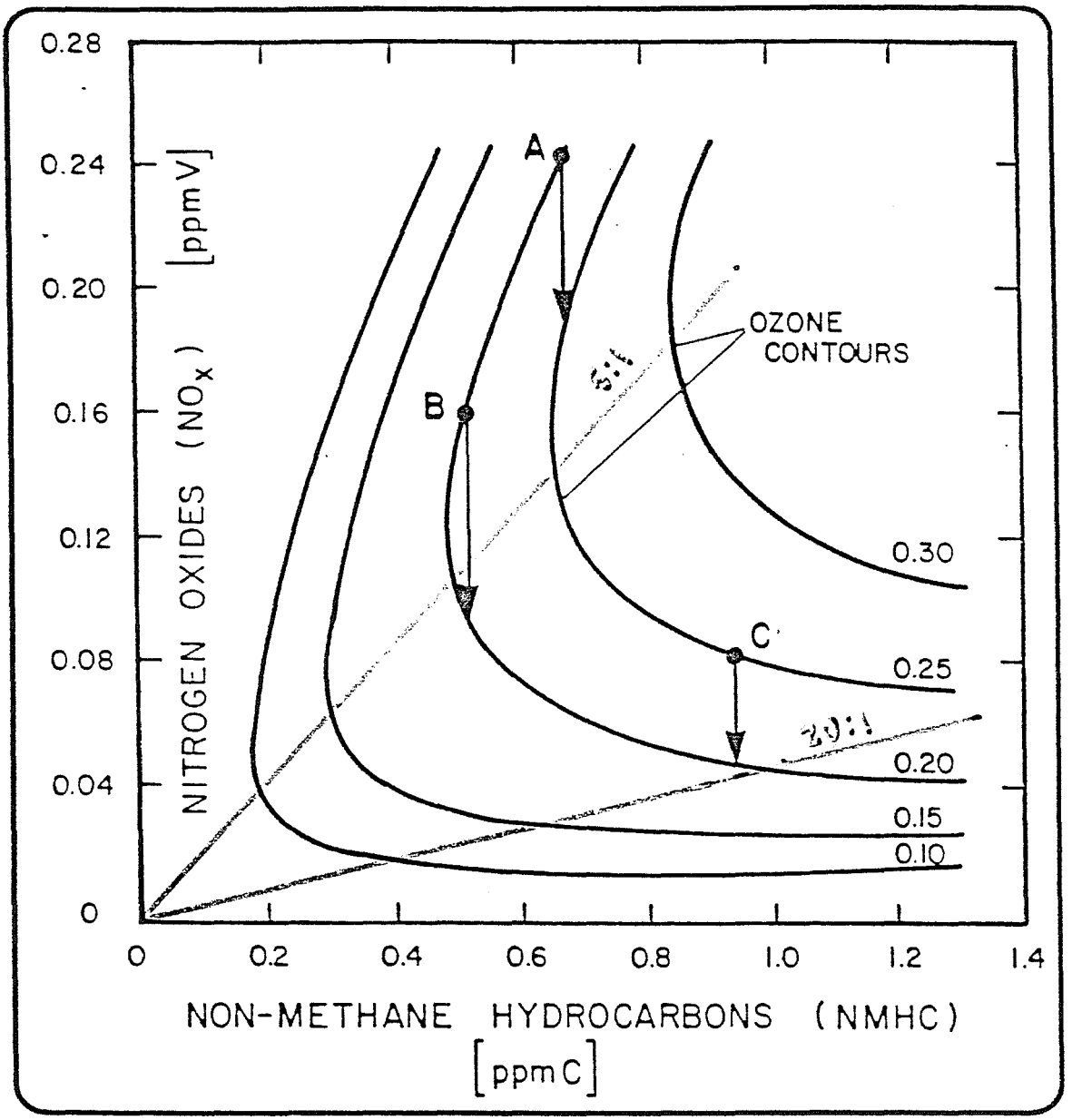
1. Simulate Episodes in Same or Adjacent Years

   Assesses model's ability to predict changes in O_3 due to changes in meteorology

2. Simulate Same Episode (pseudo-Episode) in Years Sufficiently Far Apart

   Assesses model's ability to predict changes in O_3 due to changes in emissions

Regulatory use requires #2. Must compare predictions to observed data. Most previous performance evaluations are of #1 type, however.



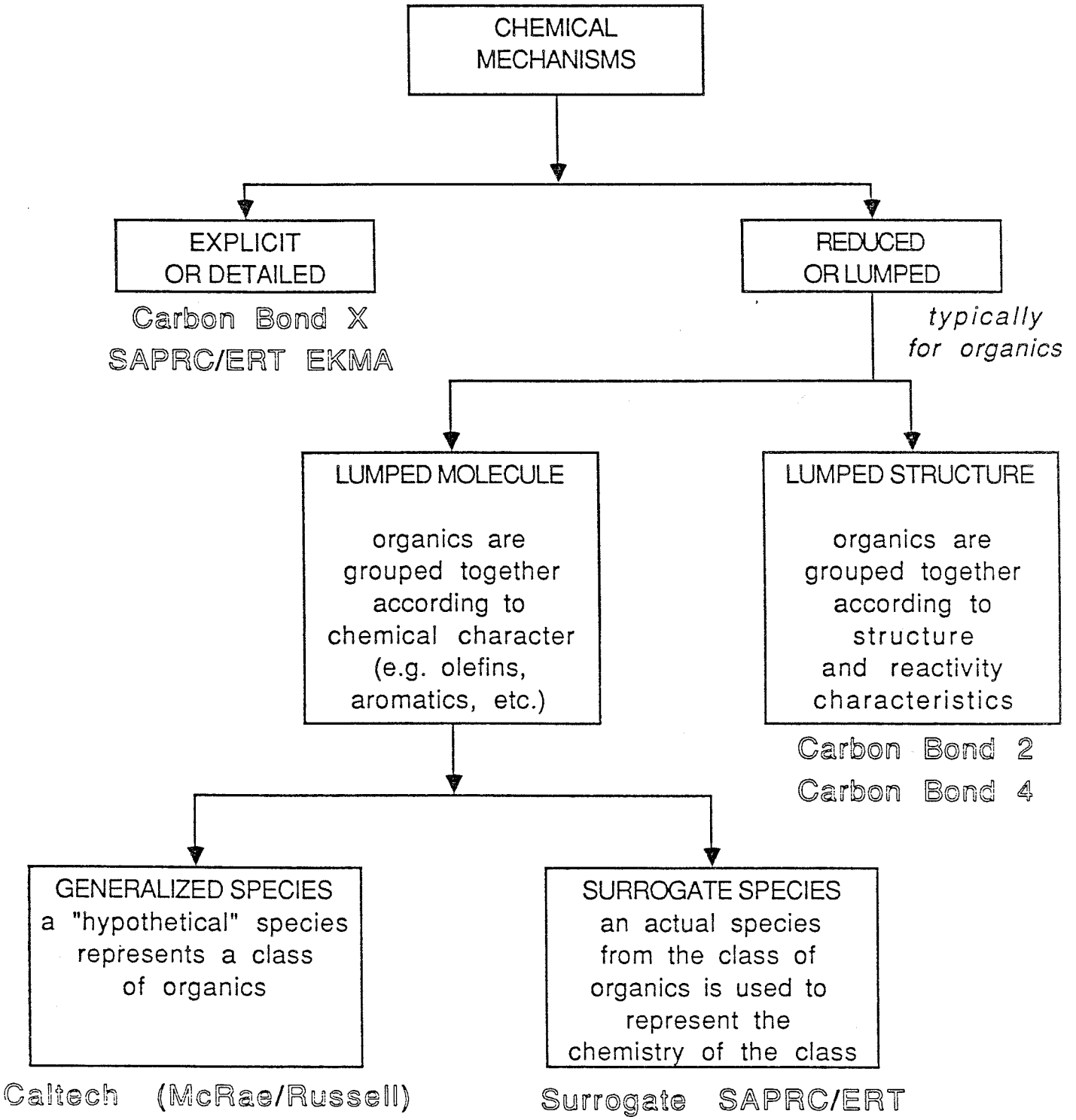
EKMA CALCULATIONS

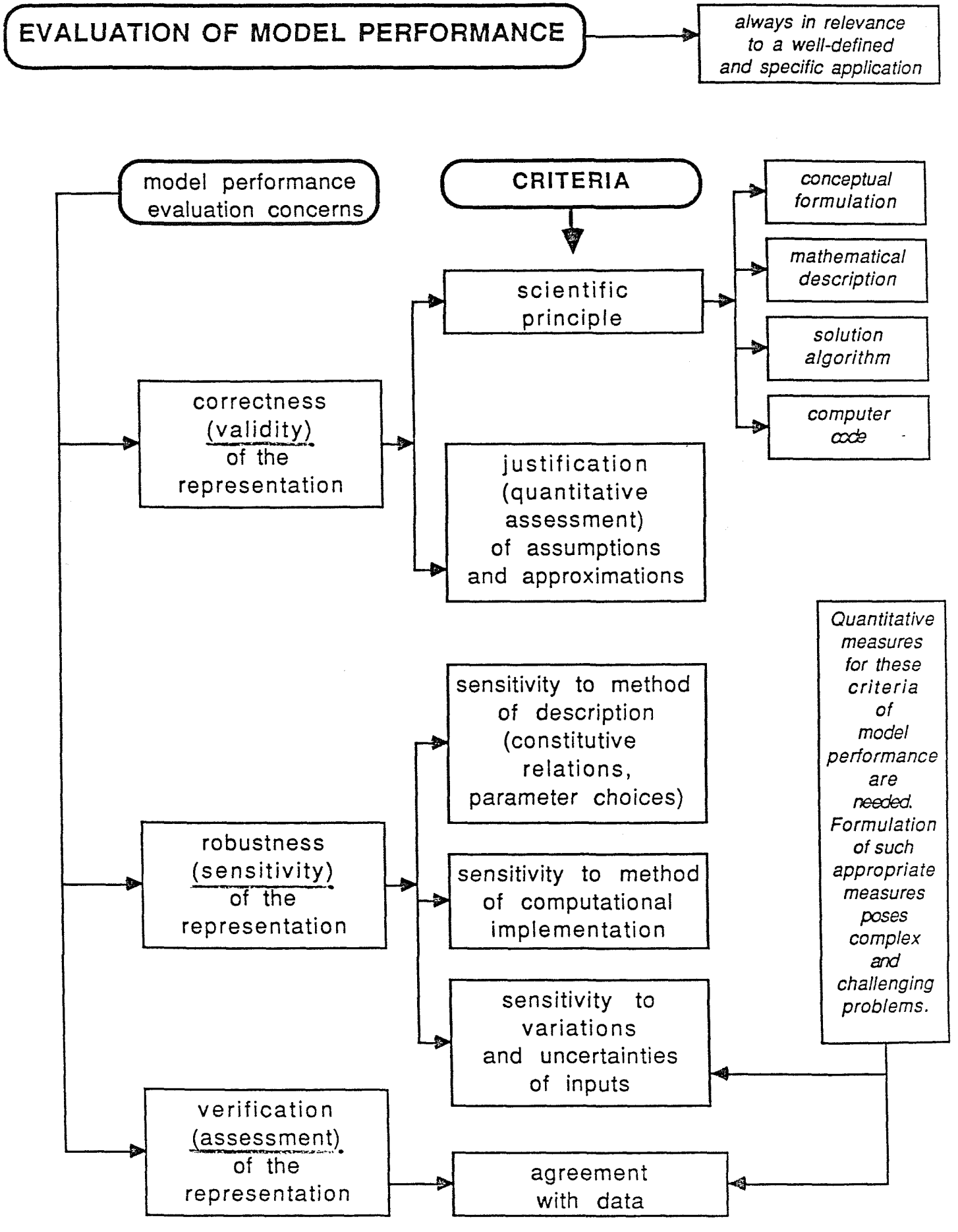
depicting the nonlinear character
of the gas phase photochemistry system

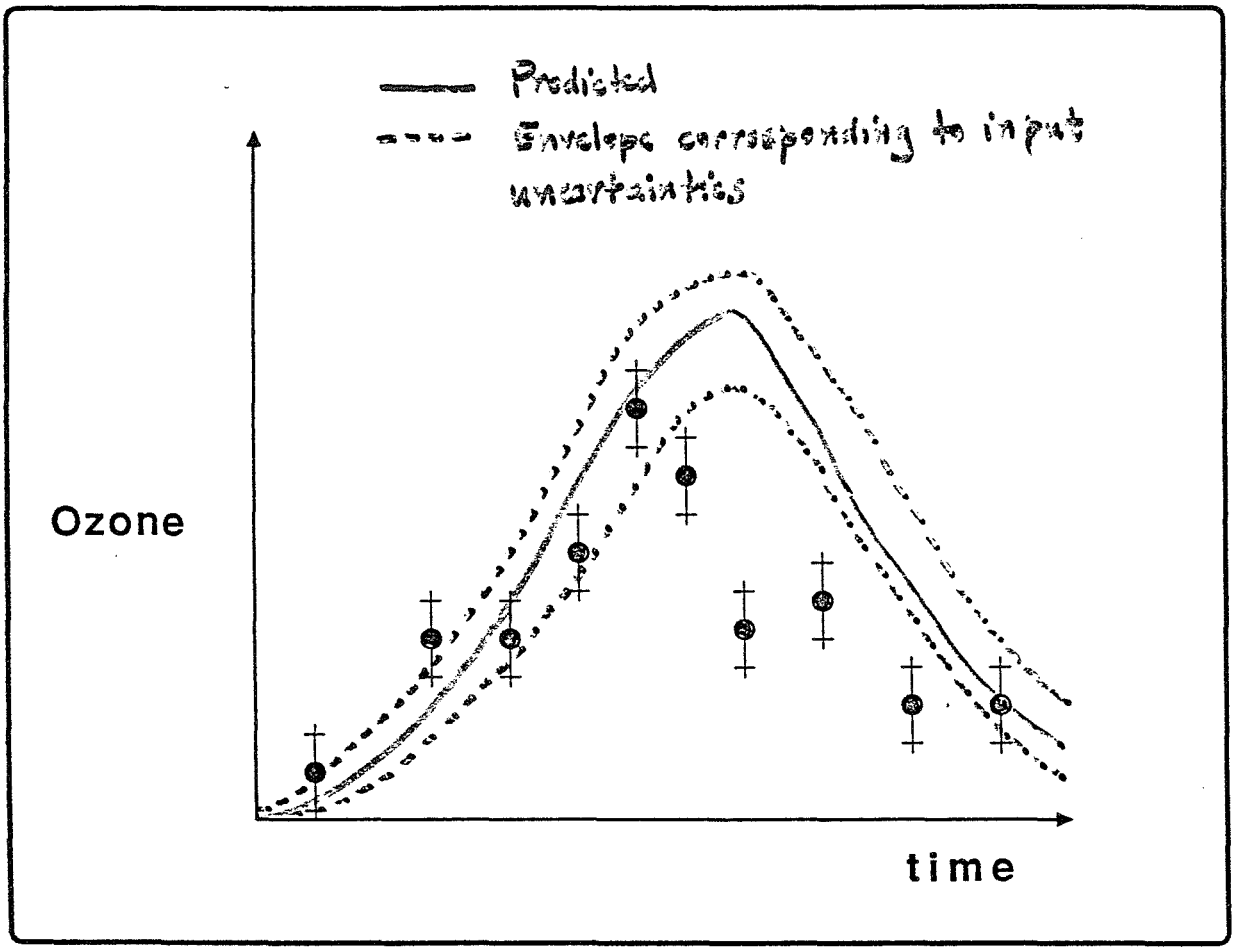
$\frac{[NMHC]}{[NO_x]}$ large (> 20) = shortage of NO that can be oxidized by RO_2. O_3 controlled by amt of NO_x available. Incr. NO_x leads to O_3 increase.

small (< 5) = ready availability of NO makes O_3 dependent on NMHC. NO will scavenge O_3 faster than $RO_2 + NO$. Also $NO_2 + OH \rightarrow HNO_3$. Incr. NO_x leads to initial decrease in O_3 and in peak. Delayed formation

GAS PHASE PHOTOCHEMISTRY
classification of mechanisms



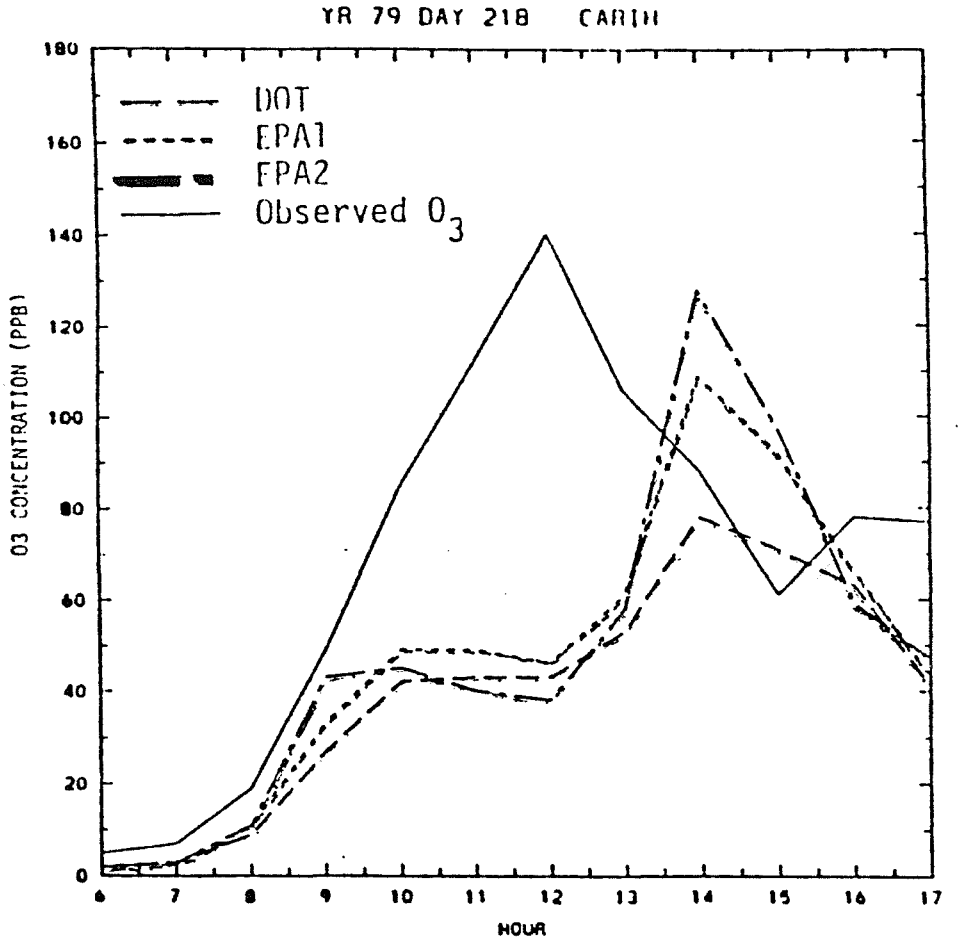

EVALUATION OF MODEL PERFORMANCE
always in relevance to a well-defined and specific application
model performance evaluation concerns
CRITERIA
conceptual formulation
mathematical description
solution algorithm
computer code
scientific principle
correctness (validity) of the representation
justification (quantitative assessment) of assumptions and approximations
sensitivity to method of description (constitutive relations, parameter choices)
robustness (sensitivity) of the representation
sensitivity to method of computational implementation
sensitivity to variations and uncertainties of inputs
Quantitative measures for these criteria of model performance are needed. Formulation of such appropriate measures poses complex and challenging problems.
verification (assessment) of the representation
agreement with data



Predicted and Observed Ozone

Key Pt - Models generally do not predict the peaks at precisely the right time and place. Want predicted peaks in the correct general area and within ± 1 hour.

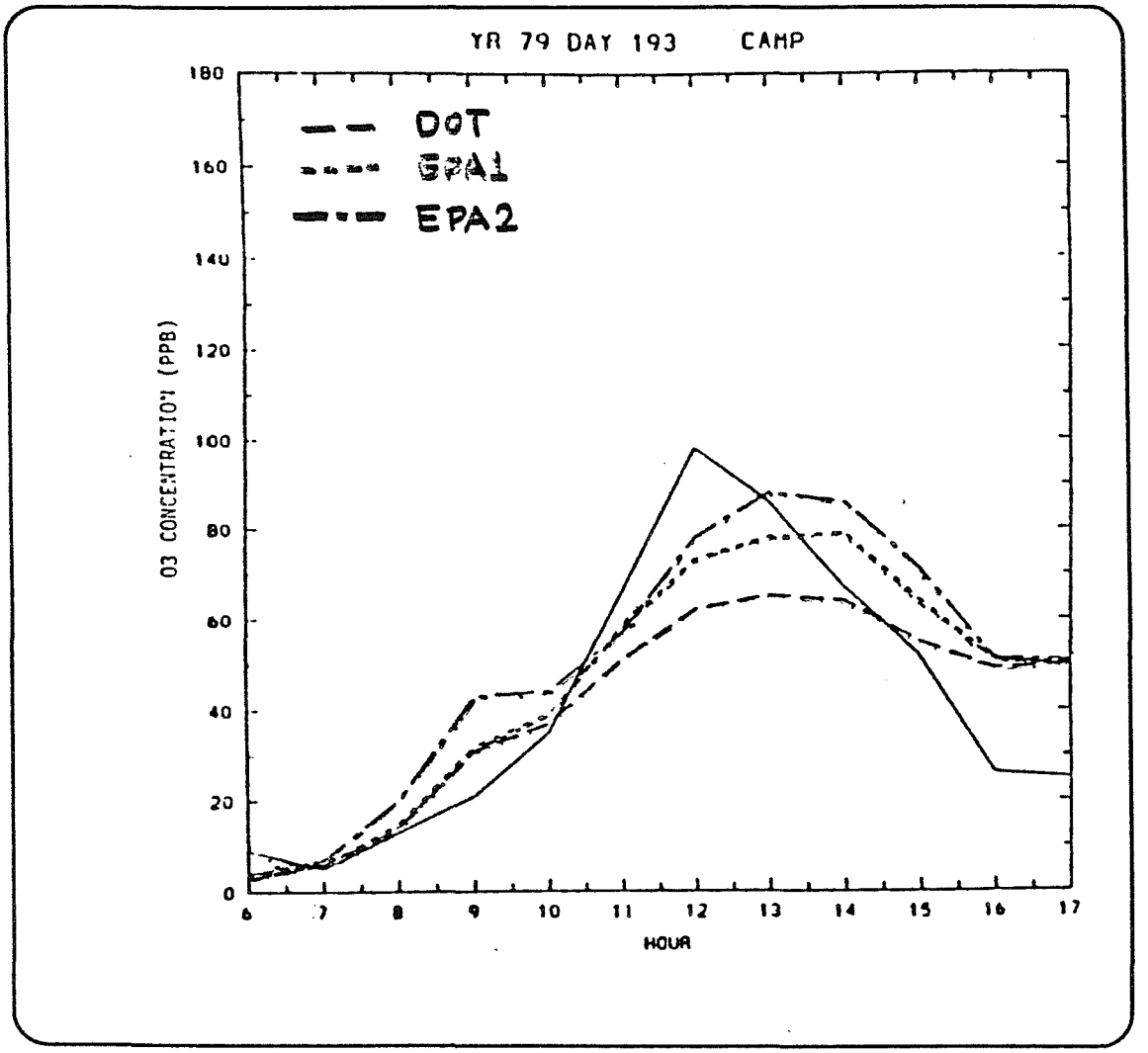
UAM (SAI)
Model Performance Evaluation (Denver, CO)
(three versions: DOT, EPA1, EPA2)



DOT to EPA1: Carbon Bond I to Carbon Bond II
EPA1 to EPA2: improvement in the numerical scheme for horizontal advection

source:

Dennis R.L. (1986) in "Air Pollution Modeling and its Application V," ed. by C. DeWispelaere, F.A. Schiermeier, and N.V. Gillani


YR 79 DAY 193 CAMP
DOT
EPA1
EPA2
03 CONCENTRATION (PPB)
HOUR
0
20
40
60
80
100
120
140
160
180
6
7
8
9
10
11
12
13
14
15
16
17

Simple Statistical Comparisons Can Be Misleading!

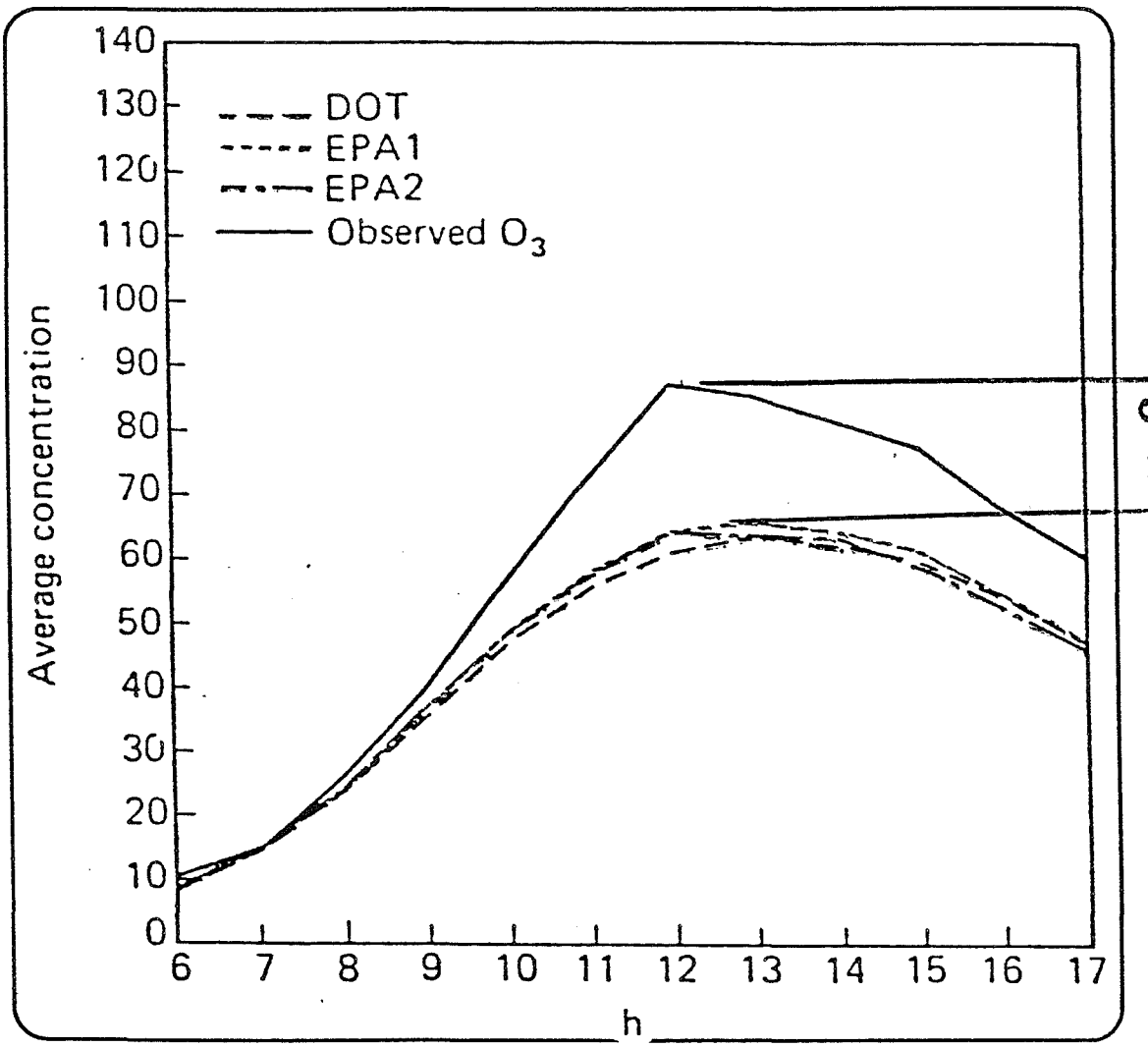
When a model does not predict the peak at the same time as the peak is observed, the effect on regulation is minimal but the effect on performance measures may be substantial and misleading.

On the previous two comparisons, inspection would lead on to prefer EPA2, because it most closely approximates observed O_3 over several peak hours. But...

Statistical Performance Measures (12-hr simulation)

	Day 79/218		Day 79/193	
	EPA1	EPA2	EPA1	EPA2
Bias (ppb)	21.9	21.3	-3.3	-8.1
Absolute deviation (ppb)	30.6	34.1	11.6	13.3

UAM (SAI)
Model Performance Evaluation (Denver, CO)
(three versions: DOT, EPA1, EPA2)



Observed and Predicted Diurnal Patterns
averaged over eleven days
and over the five monitoring sites

source:
Dennis R.L. and M.W. Dawnton (1984) in
Atmospheric Environment, 18, 2055-2069

WHY HAVE PHOTOCHEMICAL MODELS GENERALLY UNDERPREDICTED PEAK OZONE?

1. CHEMICAL MECHANISMS ARE MISSING MAJOR COMPONENTS

   UNLIKELY

2. BOUNDARY AND ALOFT CONCENTRATIONS ARE HIGHER THAN ESTIMATED

   POSSIBLE - BUT MAY NOT HAVE THAT LARGE AN EFFECT

3. ROG EMISSIONS ARE UNDERESTIMATED

   QUITE LIKELY

4. REACTIVITY OF ROG MIX IS UNCERTAIN AND UNDERESTIMATED

   QUITE LIKELY

(IN SOCAB EMISSION AND AIR QUALITY TRENDS DO NOT AGREE.)

MAJOR QUESTIONS FOR THIS CONFERENCE

PHOTOCHEMICAL AIR QUALITY MODELS ARE THE ONLY MEANS TO PREDICT PEAK OZONE CHANGES DUE TO ROG AND NO_x EMISSION CHANGES.

1. HOW ACCURATELY CAN THESE MODELS PREDICT ΔO_3 IN RESPONSE TO ΔROG AND ΔNO_x ? OR WHAT IS THE RISK OF OBTAINING THE "WRONG" ANSWER ?

2. SPECIFICALLY, REDUCTIONS OF NO_x CAN BOTH INCREASE AND DECREASE O_3 DEPENDING ON THE SITUATION. WHAT IS THE RISK THAT MODELS WILL NOT ACCURATELY PREDICT THE RELATIVE BENEFITS OF ROG AND NO_x CONTROL ?

The Case for Improved Inventories for Photochemical Modeling

W.R. Oliver
Radian Corporation
Sacramento, CA

February 1, 1988

Emission Inventory Components

- **Emission factors, activity data**
- **Location in 3-D space**
- **Time-based considerations**
- **VOC, NO_x speciation**
- **Future projections of growth, control**

Inventories for Photochemical Models

- Inventories are large data bases
- 50,000 lines of computer code
- Derived from many inputs
  - Statewide data base (EDS)
  - VOC speciation profiles
  - Stack data
  - Projection factors
- Results
  - Gridded, hourly values for individual emission species

Emission Inventories are neither "adequate" nor "inadequate." Instead, they possess varying levels of uncertainty in their components.

Expected Variability in Emissions

- **Daily variations in production levels**
- **Changes in control efficiency**
- **Seasonal effects on operations**
- **Effects from ambient temperature changes**

First, must get our "house in order:"

- **Check inventory data bases thoroughly**
- **Follow established procedures**
- **Such errors (biases) are correctable**
- **More important than normal variability**

Total Uncertainties in Inventories

- **Systematic uncertainties**
- **Random errors**
- **Double counting of facilities**
- **Missing source categories**
- **Operating deviations**

Examples:

- **Updated VOC speciation profiles can affect reactivity greatly**

- **Uncertainty in motor vehicle evaporative emissions -- ±30%**

- **Total uncertainty in SOCAB inventory -- 20 to 30%**

Recommendations

- **Increased attention on inventories for photochemical modeling is warranted.**
  - **Comparison to other data sets**
  - **Planned approach**
  - **Funding levels**

Recommendations (continued)

- **Inventory specialists must be cautious not to always "believe" their numbers.**

- **Emerging trends need to be nurtured.**

Recommendations (continued)

- **Decision makers must insist that sufficient time and resources are given to examining inventory data bases for errors before the data set is used.**

MIKE NAZEMI
SOUTH COAST AIR QUALITY
MANAGEMENT DISTRICT

HOW TO OBTAIN ACCURATE EMISSIONS INVENTORIES

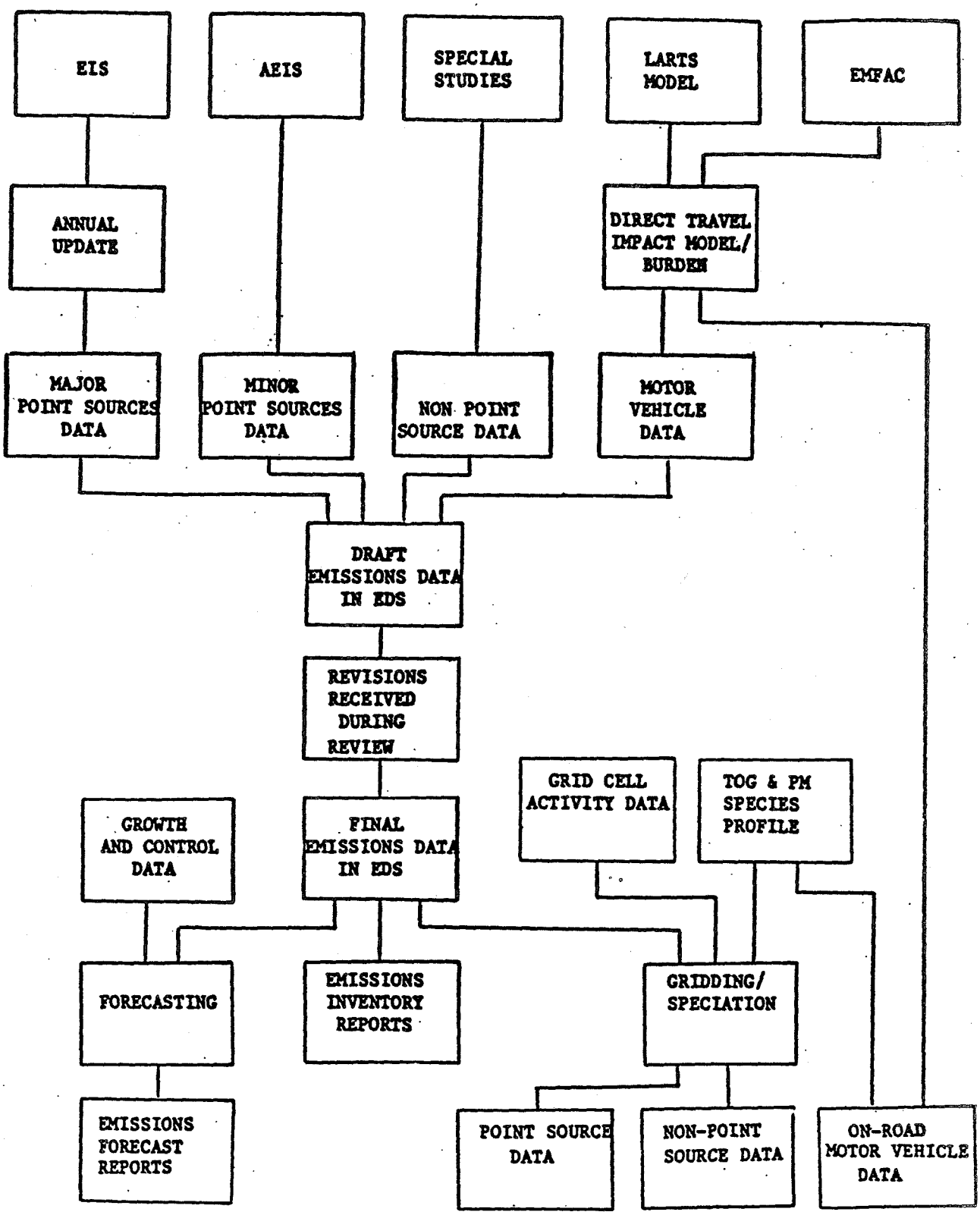
MEASURE EVERY SOURCE

CANNOT BE DONE

- 12 MILLION PEOPLE
- 8 MILLION VEHICLES
- 13,350 SQUARE MILES
- 55,000 PERMITTED STATIONARY UNITS
- 200 NON-PERMITTED AREA SOURCE CATEGORIES

OVERVIEW OF EMISSIONS DATA DEVELOPMENT

IN THE SOUTH COAST AIR BASIN



QUALITY OF THE PHOTOCHEMICAL EMISSIONS INVENTORY
FOR THE SOUTH COAST AIR BASIN

	EMISSION FACTORS	ACTIVITY DATA	TEMPORAL VARIATIONS	SPATIAL VARIATIONS	VOC SPECIATION	UNCERTAINTY IN TOTAL EMISSIONS
MAJOR POINT SOURCES (e.g. POWER PLANTS, REFINERIES)	STRONG	STRONG	STRONG	STRONG	MODERATE	SMALL
MINOR POINT SOURCES	GOOD TO MODERATE	POOR	POOR	MODERATE	MODERATE	LARGE
AREA SOURCES	MODERATE	MODERATE	MODERATE	POOR	POOR	LARGE
MOTOR VEHICLES (INCLUDING HDVs)	MODERATE	MODERATE	POOR	POOR	MODERATE	LARGE

IMPORTANCE PLACED UPON EMISSIONS DATA

SCAQS BUDGET ▪ APPROX. $10 M

EMISSIONS INVENTORY PORTION ▪ APPROX. $400K

CURRENT IMPROVEMENTS

UNINVENTORIED SOURCES IDENTIFIED

+ ARB CONTRACT AWARDED TO RANK THESE SOURCES
- NEED MUCH LARGER CONTRACT TO QUANTIFY & TO GRID

UNCERTAINTY ISSUE RECOGNIZED

+ SMALL ARB CONTRACT AWARDED TO ADDRESS THE ISSUE
- NEED EXTENSIVE AMOUNT OF DATA COLLECTION TO ADDRESS ALL SOURCES

SCAQS DAY SPECIFIC EMISSIONS DATA

+ DATA COLLECTED (NOT ANALYZED)
- LIMITED DATA

SMALL VOC SOURCES:

+ ARB CONTRACT AWARDED TO IMPROVE A SIGNIFICANT PORTION OF AREA SOURCES (IN INITIAL STAGES)

CURRENT IMPROVEMENTS (CONT.)

MOTOR VEHICLE EMISSION FACTORS

+ BEING UPDATED

- NOT FAST ENOUGH

MOTOR VEHICLE ACTIVITY DATA

+ SMALL DISTRICT/MVMA CONTRACT WILL BE AWARDED FOR TRUCK DATA

- VERY LIMITED STUDY NEED MORE MONEY

GENERAL NEEDS

- CHANGE ATTITUDE TOWARDS UNCERTAINTY
  + DOES NOT CANCEL -
- SET PRIORITY ON EMISSIONS DATA
- INCREASE BUDGET
- MORE COOPERATION AMONG AGENCIES
- ALLOW TIME TO DEVELOP DATA
- DEVELOP COMPREHENSIVE PLAN
- DO IT ONCE, CORRECTLY

SPECIFIC NEEDS
IMPROVE:

- MV EMISSION FACTORS
- MV ACTIVITY DATA
  - -BY TYPE (LDA & HD)
  - -SPATIAL
  - -TEMPORAL
- UNINVENTORIED SOURCES
  - -IDENTIFY
  - -QUANTIFY
- UNCERTAINTIES
  - -COLLECT MORE DATA
- MINOR POINT SOURCES
  - -HIRE ADDITIONAL STAFF TO UPDATE

GARY HONCOÓP
CALIFORNIA AIR RESOURCES
BOARD

COMPARING NMOC:NOx AMBIENT RATIOS WITH ROG:NOx EMISSION RATIOS

Hydrocarbons (Generic)

≠

Organic Compounds (EPA)

HYDROCARBONS/ORGANIC COMPOUNDS

Nonreactive	Reactive
Methane	Reactive Hydrocarbons Nonmethane Hydrocarbons Reactive Organic Gases Nonmethane Organic Compounds

ORGANIC COMPOUNDS

Ambient Concentrations = NMOC

Emissions = ROG

$NO_X = NO_2 + NO$

OXIDES OF NITROGEN = **NITROGEN DIOXIDE** + **NITRIC OXIDE**

NITROGEN OXIDES

Ambient Concentrations = NOx

Emissions = NOx

RATIOS

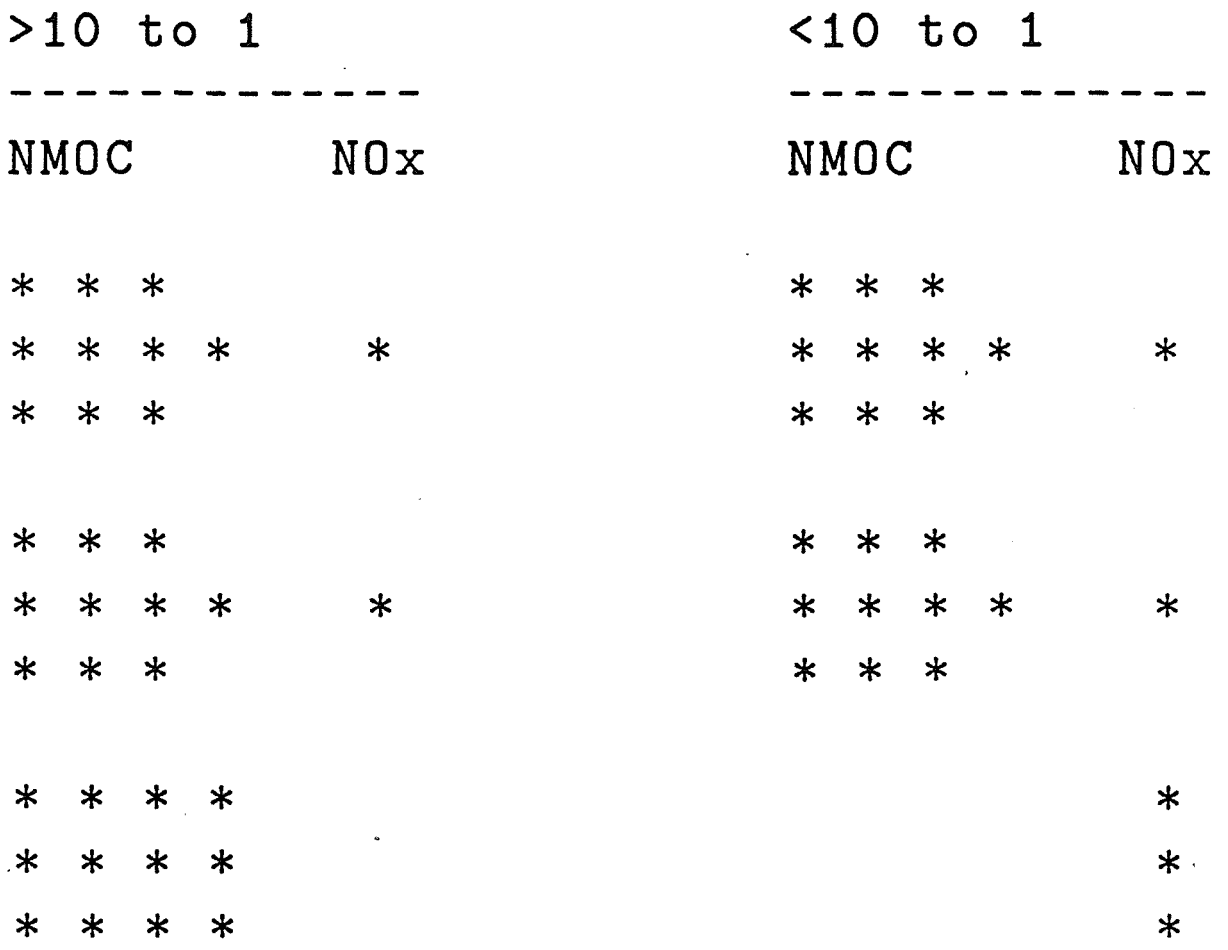
An expression of the proportional relationship of the amount of one item to another.

USES FOR RATIOS

1. Input to EKMA models
2. Check model performance
3. Assess which emission is limiting

CONCEPT OF LIMITING EMISSION

(assume ratio of 10 to 1)



REASONS FOR DIFFERENCES BETWEEN EMISSION AND AMBIENT RATIOS

REASONS FOR DIFFERENCES

1. Ratios calculated with different units
2. Spatial differences
3. Temporal differences
4. Uncertainty in NMOC measurements
5. Meteorological effects
6. Anthropogenic emissions only
7. Chemical transformation of emissions

SAMPLE RATIOS
FROM
SELECTED AREAS IN CALIFORNIA

RATIOS FOR CENTRAL KERN COUNTY

ROG:NOx EMISSION RATIOS[1]		NMOC:NOx AMBIENT RATIOS[2]	
All Sources	: 3.3	Composite Mean	: 21.8
Mobile Sources	: 1.3	Bakersfield	: 22.9
Stationary Sources	: 4.5	Oildale	: 20.7
Stationary Sources, but without Power Plants	: 4.5		

---

1. Based on 1984 average annual day emissions for Central Kern County
2. Based on 1984-1986 July-Sept. daily mean concentrations

RATIOS FOR VENTURA COUNTY

ROG:NOx EMISSION RATIOS[1]		NMOC:NOx AMBIENT RATIOS[2]	
Statewide Ratio	3.5	Composite Mean	17.6
South Central Coast Air Basin Ratio	4.4		
County-All Sources	4.0		
Stationary Sources	5.9		
Mobile Sources	2.4		
Range of Ratios for 2 X 2 km grids around Ventura[3]	2-100		

---

1. Based on 1985 Countywide emissions for average annual day
2. Based on 1984-1986 July-Sept. daily mean concentrations
3. Based on September 12, 1985, gridded emission inventory

WAYS TO IMPROVE AGREEMENT BETWEEN AMBIENT AND EMISSION RATIOS

WAYS TO IMPROVE

1. Improve ambient NMOC data
2. Increase NMOC monitoring
3. Improve emission inventories

WHAT TECHNIQUES ARE AVAILABLE FOR GENERATING WINDFIELDS?

R. C. KESSLER

What do we mean by "windfield"?

Horizontal winds defined at 500-3000 grid locations at 4 to 10 vertical levels every hour.

Horizontal winds are external input to photochemical grid model. Photochemical model computes vertical winds.

To generate a windfield, we utilize numerical techniques to combine

Observations

- surface
- upper-air

- routine observations
- observations from intensive measurement programs

Knowledge of meteorological processes

- theory
- empirical information

General classification of numerical techniques

Objective analysis

Diagnostic wind models

Prognostic models

Choice of technique depends on the spatial and temporal representativeness of available observations

OBJECTIVE ANALYSIS

Mathematical combination of observations.

interpolation
extrapolation

No physics

Major assumption:

Available observations completely represent the airflow within the domain of the photochemical model.

Advantages:

Computationally inexpensive

Disadvantages

Available observations are frequently unrepresentative of airflow in certain portions of a domain. This is especially true in regions of complex terrain.

DIAGNOSTIC WIND MODELS

Relatively simple estimation of complex terrain effects

- channeling and deflection of flow by terrain
- slope flows

Can be combined with objective analysis of observations

- approach #1
  - do objective analysis of available observations
  - adjust objectively analyzed field for terrain effects
- approach #2
  - estimate terrain effects on "mean" flow--"first guess" field
  - incorporate "first guess" field and available observations into objective analysis

Advantages:

- May require fewer observations than simple objective analysis to produce credible wind field.
- Computationally inexpensive.

Disadvantages

- In the absence of representative observations, diagnostic wind models cannot by themselves generate certain airflow features important to air quality simulation
  - sea breezes
  - low-level jets
  - terrain-generated mesoscale eddies

PROGNOSTIC MODELS

Numerical solution of the governing equations of the atmosphere

Required information

- initial state of atmosphere within domain
- "forcing" of domain-scale flow by large-scale processes

Model simulates response of airflow to

- differential surface heating
  - sea breeze
- complex terrain
  - thermodynamic upslope and downslope flows
  - blocking and deflection of airflow by terrain
  - mesoscale eddies

Advantages:

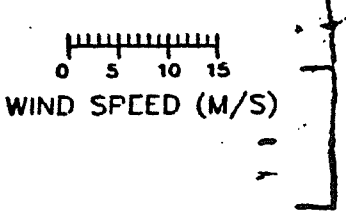
- All relevant physical processes simulated
- Does not require significant observational input. This is especially important in representation of upper-air winds, for which representative observations are frequently unavailable.
- In addition to wind field, temperature field is simulated. Thus prognostic model could supply mixing height and stability information to photochemical model.

Disadvantages

- Computationally expensive (relative to other methods)
- Does not necessarily reproduce available observations.

EXAMPLE

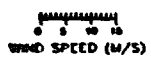
Following are five different representations of the surface airflow in the Ventura-Santa Barbara area at 1200 PDT on 23 September 1985.



a) Subjective streamline analysis superimposed upon plot of surface wind observations.

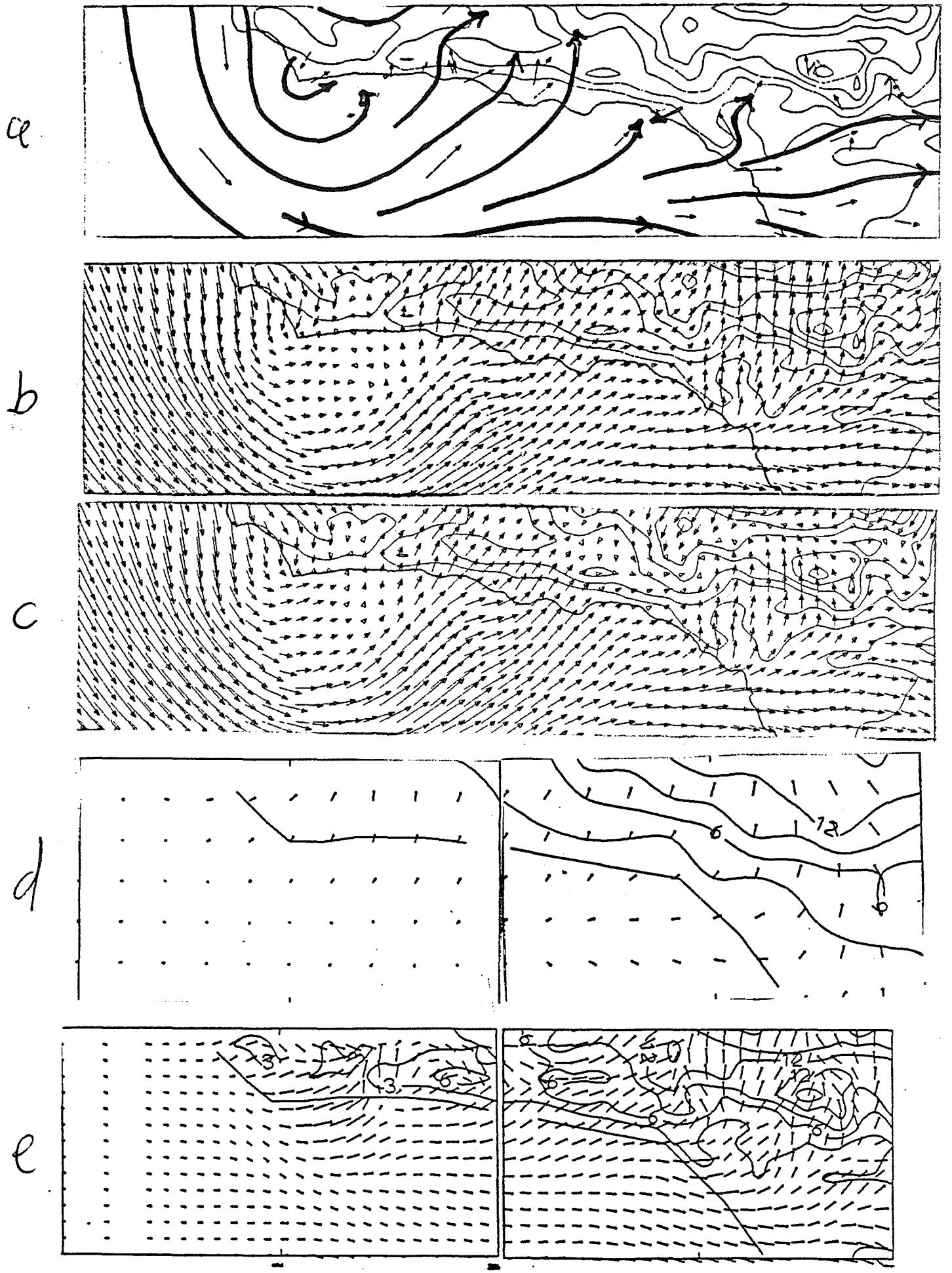
b) Gridded objective analysis of surface wind observations. Grid resolution is 4 km.

c) Gridded wind field generated by SAI diagnostic wind model. Grid resolution is 4 km.



d) Wind field generated by coarse-grid primitive-equation simulation. Grid resolution is 10 km.

e) Wind field generated by fine-grid primitive-equation simulation. Minimum grid resolution is 4 km.


a
b
c
d
e
6
12
3
6
3
6
12
6
6

FINAL POINTS

Objective analysis is an inexpensive technique. However, collection of sufficient observational data for a valid objective analysis can be very expensive.

Diagnostic wind models may improve representation of airflow over complex terrain. However, they are currently unable to represent certain important airflow patterns; there seems little prospect for improvement of these models at this time.

Prognostic models show promise in providing valid representations of airflow in the absence of representative observations. Although prognostic meteorological modeling is computationally much more expensive than objective analysis or diagnostic wind modeling, it may be considerably less expensive than intensive upper-air observations sufficient for valid objective analysis.

However, for prognostic models to be credible, model output must be verified against available observations where possible. Prognostic model verification efforts are currently under way in the South Central Coast and South Coast Air Basins.

More research is needed in methods of combining prognostic models and observations. We would expect such an approach to produce the best possible windfields for photochemical air quality models.

WIND FIELD UNCERTAINTY AND PHOTOCHEMICAL MODELING

BY

KIT K. WAGNER

AIR QUALITY MODELING SECTION
TECHNICAL SUPPORT DIVISION
CALIFORNIA AIR RESOURCES BOARD

PRESENTED AT

PHOTOCHEMICAL MODELING AS A TOOL FOR DECISION MAKERS

February 1-3, 1988 at the California Institute of Technology

QUESTIONS

WHAT IS THE ROLE OF WIND ANALYSIS IN PHOTOCHEMICAL MODELING?

WHAT ARE THE ACCURACY REQUIREMENTS FOR WINDS USED FOR PHOTOCHEMICAL MODELING?

WHAT METHODS CAN BE USED TO DETERMINE THE ACCURACY OF WIND ANALYSES?

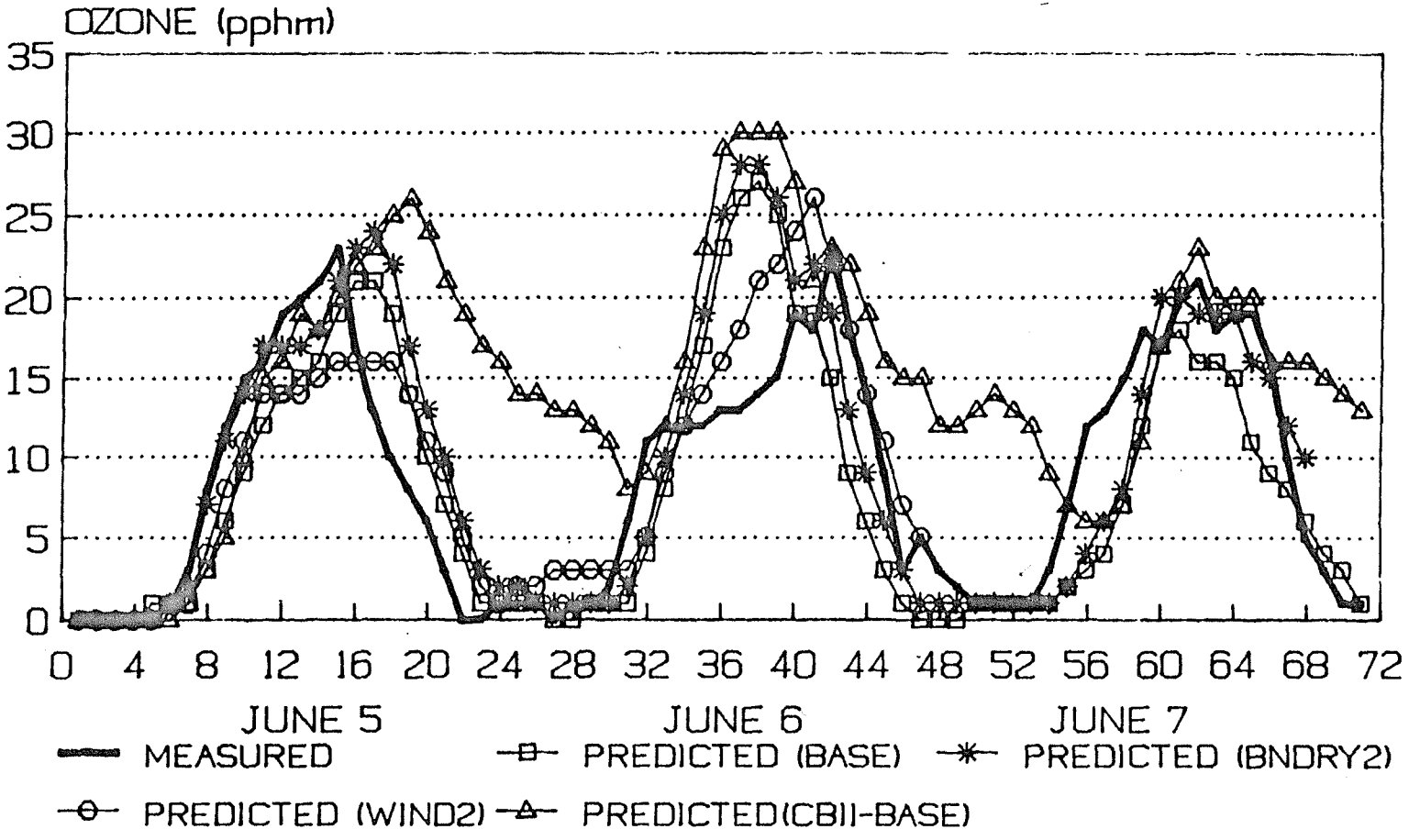
HOW ACCURATE ARE THE CURRENT WIND ANALYSIS METHODS?

WHAT ARE THE PROSPECTS OF IMPROVING PHOTOCHEMICAL MODELING BY IMPROVING WIND ANALYSES?

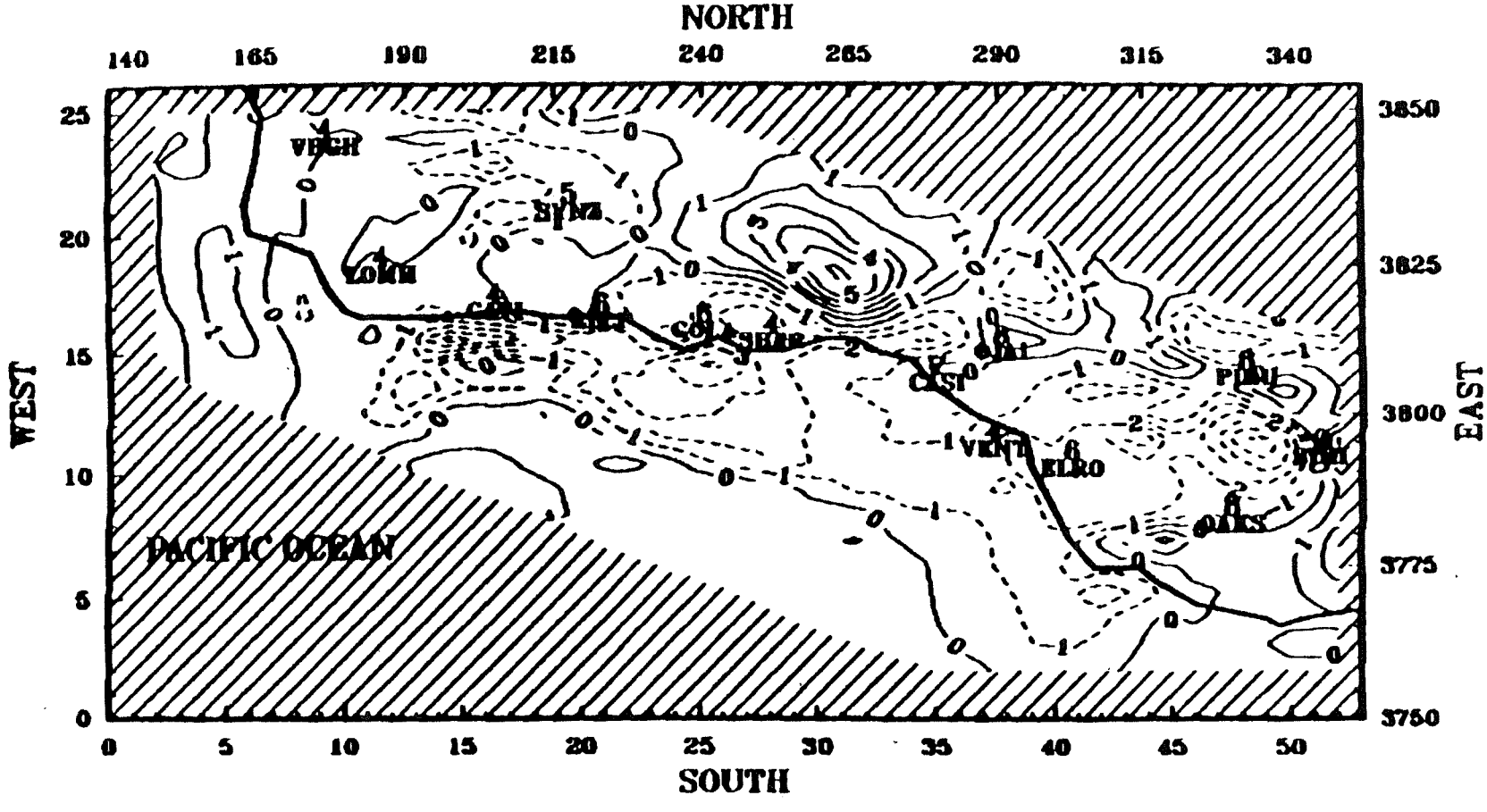
PHOTOCHEMICAL MODELS REQUIRE AN ANALYZED WIND FIELD WHICH IS USED TO MOVE POLLUTANTS AND EMISSIONS FROM PLACE TO PLACE WITHIN THE MODELING AREA.

STUDIES HAVE SHOW THAT PHOTOCHEMICAL MODELING RESULTS CAN CHANGE IF THE INPUT WIND FIELD CHANGES.

COMPARISON OF MEASURED AND PREDICTED OZONE AT SAN BERNARDINO JUNE 5-7, 1985



SCE



Ozone Deficit-Enhancement Plot for 16 September 1984 in the South Central Coast Air Basin.
(Caltech Wind Fields Minus Diagnostic Windfields; pphm)

RADIAN

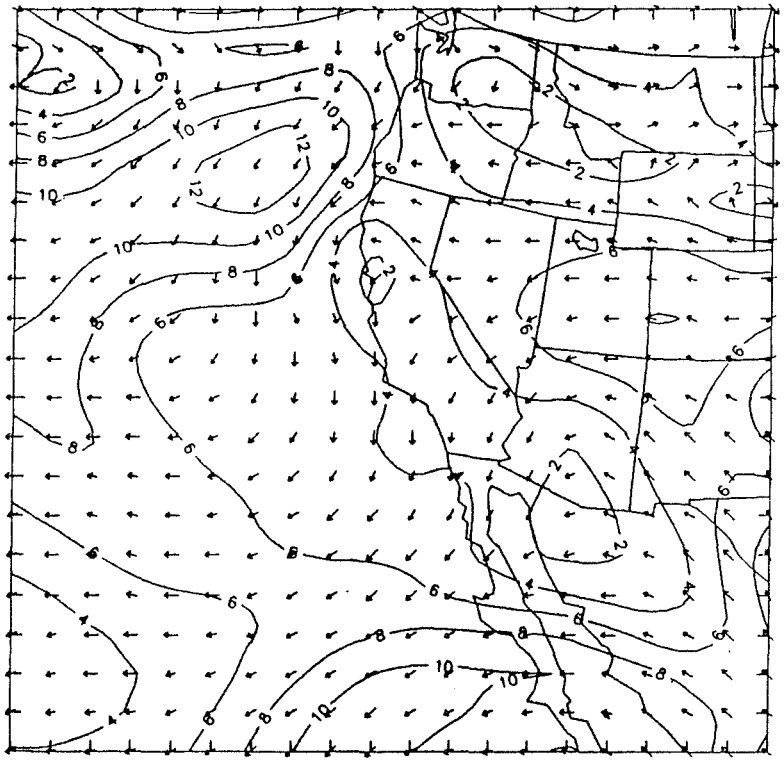
THE AMOUNT OF CHANGE IN PHOTOCHEMICAL MODELING RESULTS DEPENDS UPON:

* THE COMPLEXITY OF THE WINDS.

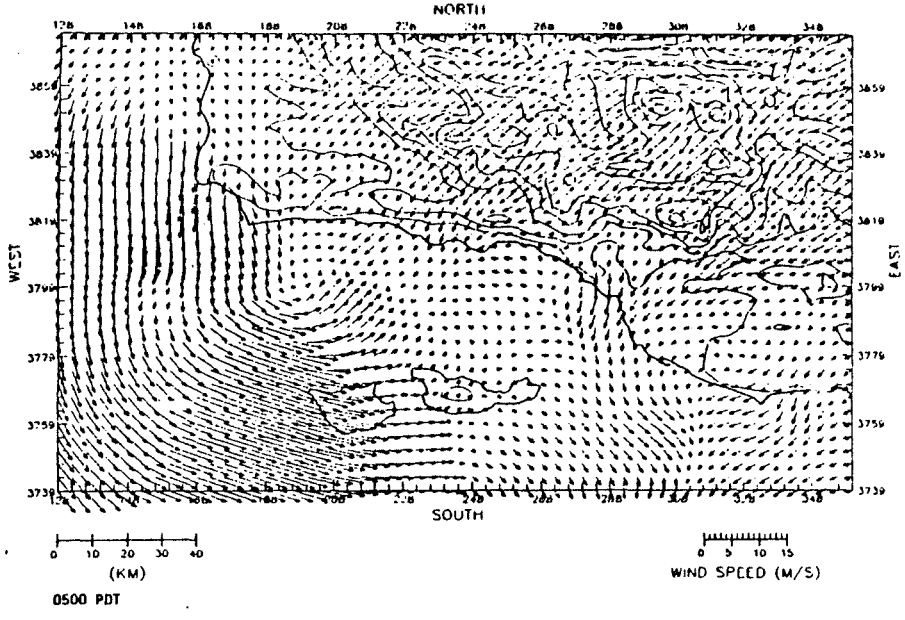
* THE VARIABILITY OF THE EMISSIONS.

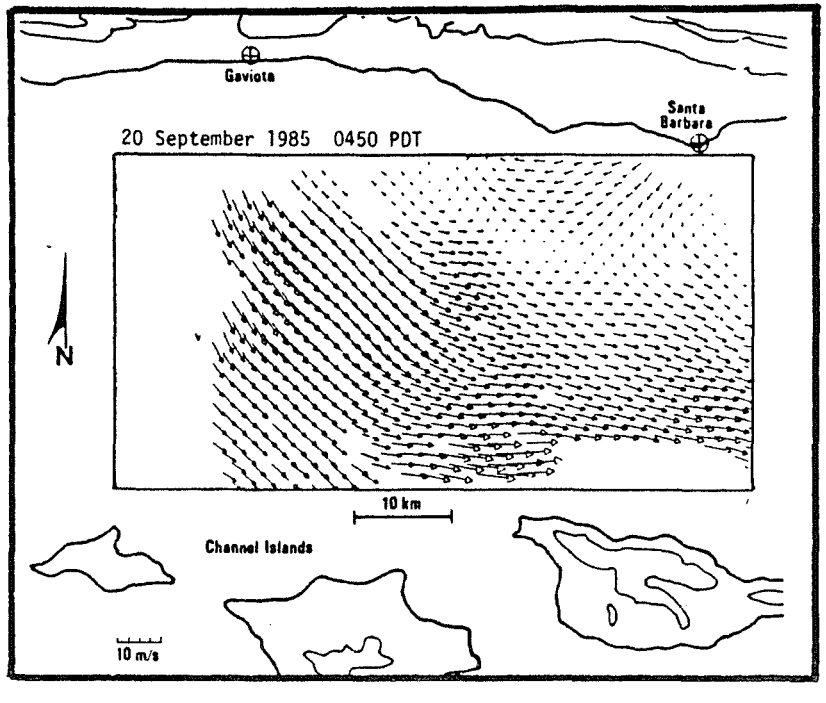
ERRORS IN THE PHOTOCHEMICAL MODELING WILL OCCUR WHEN ERRORS IN THE WIND ANALYSIS CAUSE POSITIONING ERRORS LARGER THAN THE VARIATION IN POLLUTANTS AND EMISSIONS.

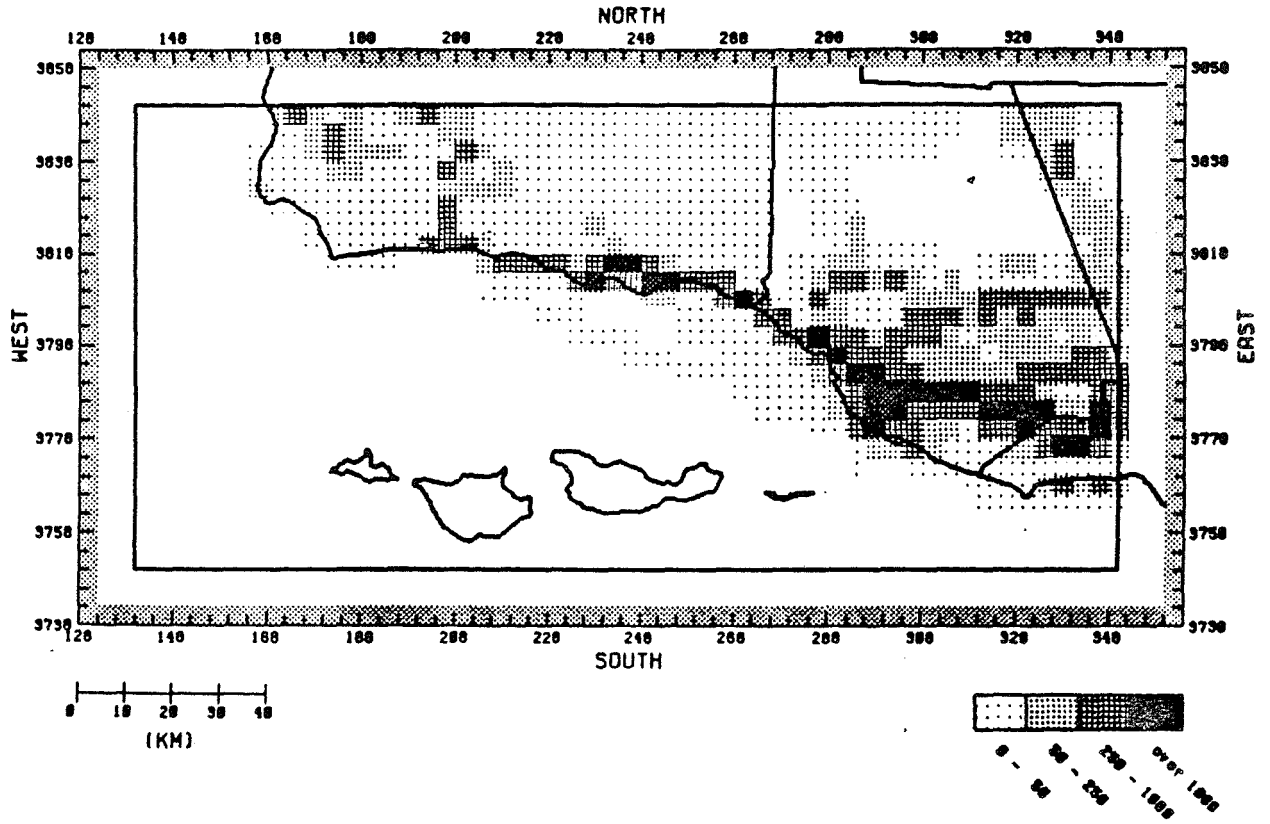
BOUNDARY LAYER WIND SPEED (m/s) 9-20-85 12 Z



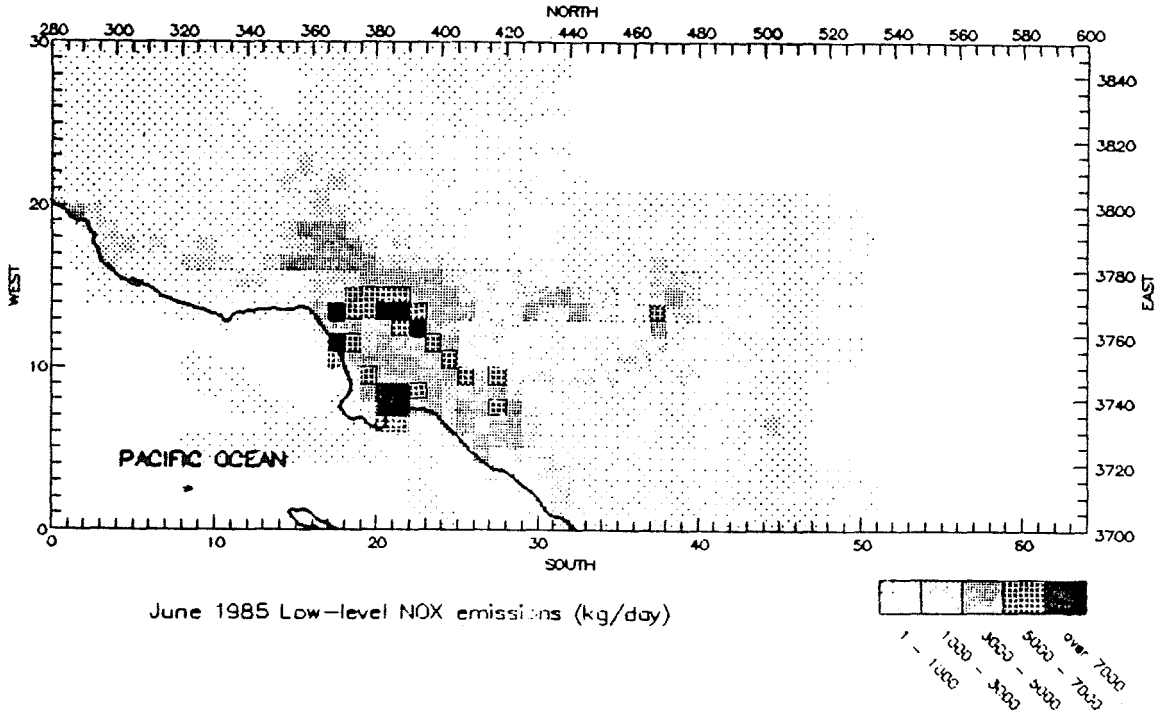
LFM Gridded Data - Boundary Layer Wind Speed (m/s)
0500 PDT - 20 September 1985.



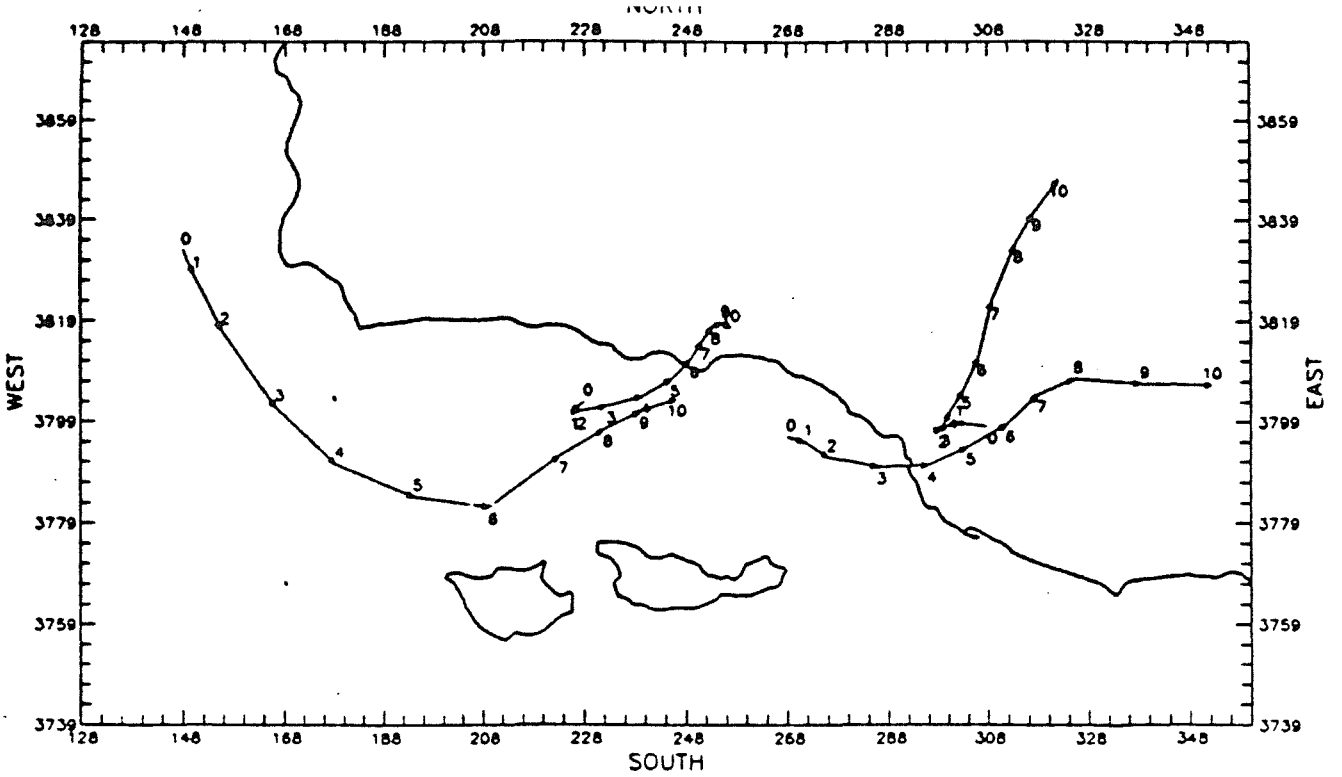




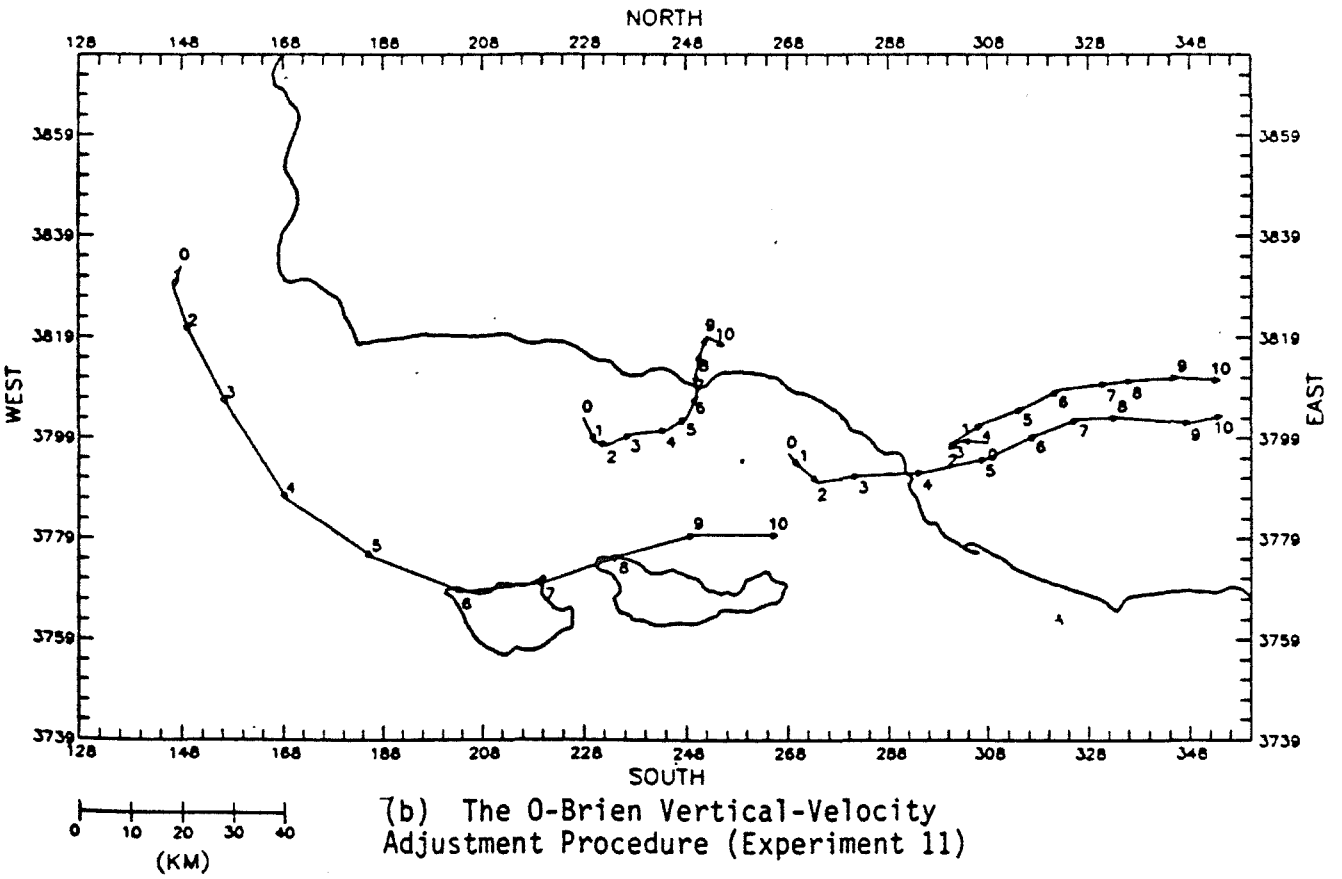
Total low-level NO_x emissions (Kg/day) for 25 September 1980.



June 1985 Low-level NOX emissions (kg/day)



(a) No Vertical-Velocity Adjustment (Experiment 10)



(b) The O-Brien Vertical-Velocity Adjustment Procedure (Experiment 11)

Example of the use of two-dimensional particle paths to compare wind fields (Kessler and Douglas, 1987). These particle paths were computed from SCCCAMP 1985 surface wind fields for 23 September 1985. In the top figure, the gridded wind fields are computed via simple objective analysis. In the bottom figure, the gridded wind fields were adjusted to be mass-consistent with an imposed vertical velocity profile. All particle paths were initiated at 0600 PDT on 23 September 1985.

WIND ANALYSES CAN BE COMPARED TO WIND OBSERVATIONS.

THE TRANSPORT OF A POLLUTANT IN A MODEL SIMULATION CAN BE COMPARED TO THE TRANSPORT OF A POLLUTANT IN THE REAL ATMOSPHERE.

AN ACCURATE WIND ANALYSIS WILL MATCH THE WIND OBSERVED IN THE ATMOSPHERE AND POLLUTANT TRANSPORT CALCULATED BY THE SIMULATION WILL MATCH THE TRANSPORT IN THE ATMOSPHERE.

AN ESTIMATE OF THE ACCURACY OF A WIND ANALYSIS METHOD CAN BE MADE BY PERFORMING SIMULATION EXPERIMENTS WITH THEORETICAL WIND PATTERNS.

CURRENT PHOTOCHEMICAL MODELING STUDIES DEFINE EMISSIONS AT A RESOLUTION OF 2 TO 5 KILOMETERS.

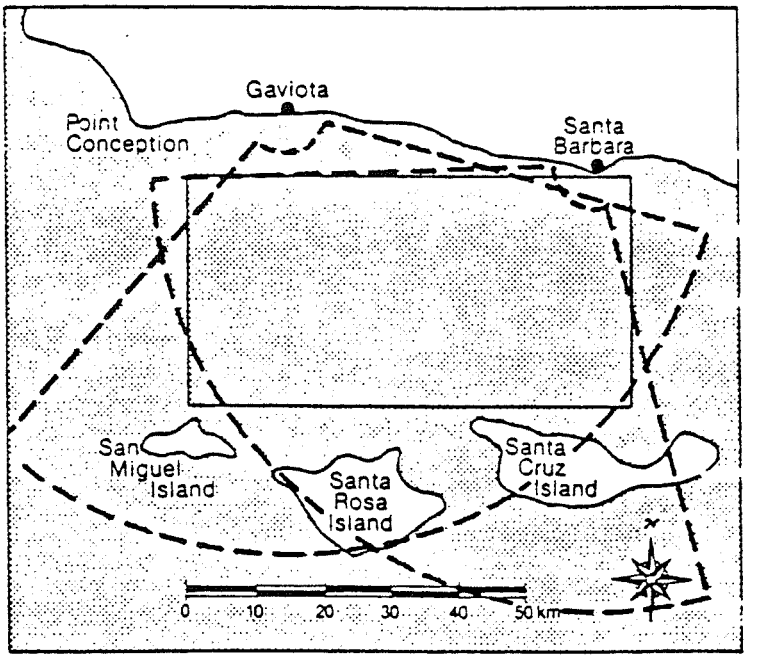
WIND INTERPOLATION ERRORS EXCEED PHOTOCHEMICAL MODELING REQUIREMENTS BECAUSE WIND OBSERVATIONS ARE TAKEN AT INTERVALS LARGER THAN 2 TO 5 KILOMETERS.

ATMOSPHERIC SIMULATION MODELS CAN ANALYZE THE WIND AT THE REQUIRED RESOLUTION. ERRORS IN WIND ANALYSES FOR PHOTOCHEMICAL MODELING HAVE NOT BEEN THROUGHLY EVALUATED.

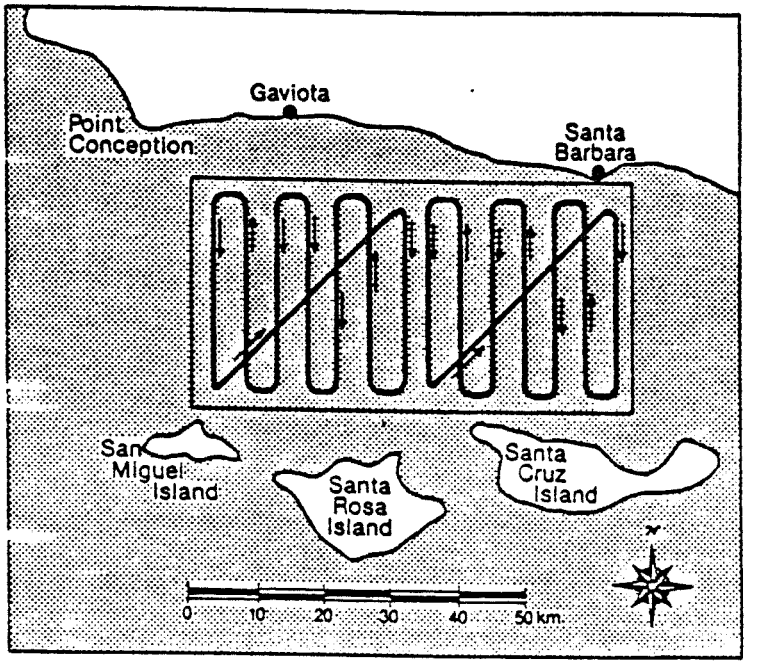
REMOTE SENSING TECHNIQUES MAY BE ABLE TO TAKE WIND OBSERVATIONS AT THE REQUIRED RESOLUTION IN THE FUTURE.

MORE THROUGH EVALUATION OF THE ERRORS IN WIND ANALYSES WITH ATMOSPHERIC MODELS IS NEEDED.

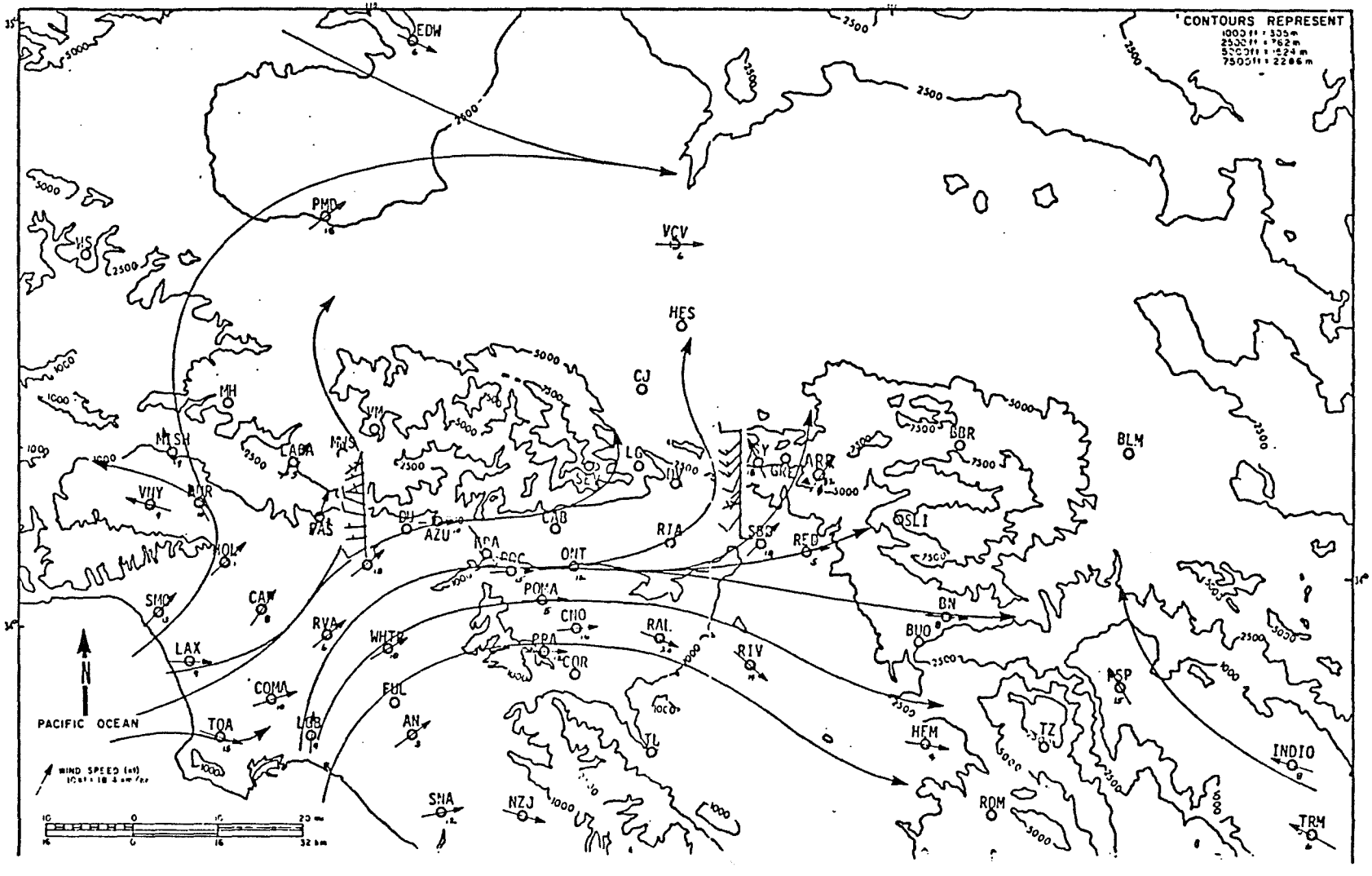
IT REMAINS TO BE DEMONSTRATED THAT IMPROVEMENTS IN WIND ANALYSIS WILL LEAD TO IMPROVEMENTS IN PHOTOCHEMICAL MODELING PERFORMANCE.



Doppler radar scan sectors used during SCCCAMP.



Grid patterns flown by the chaff-release aircraft during SCCCAMP.



♦ Skyforest
▲ Strawberry Mt. Lookout

Fig. III-7. STREAMLINES FOR 1600 PDT on 8/16/73

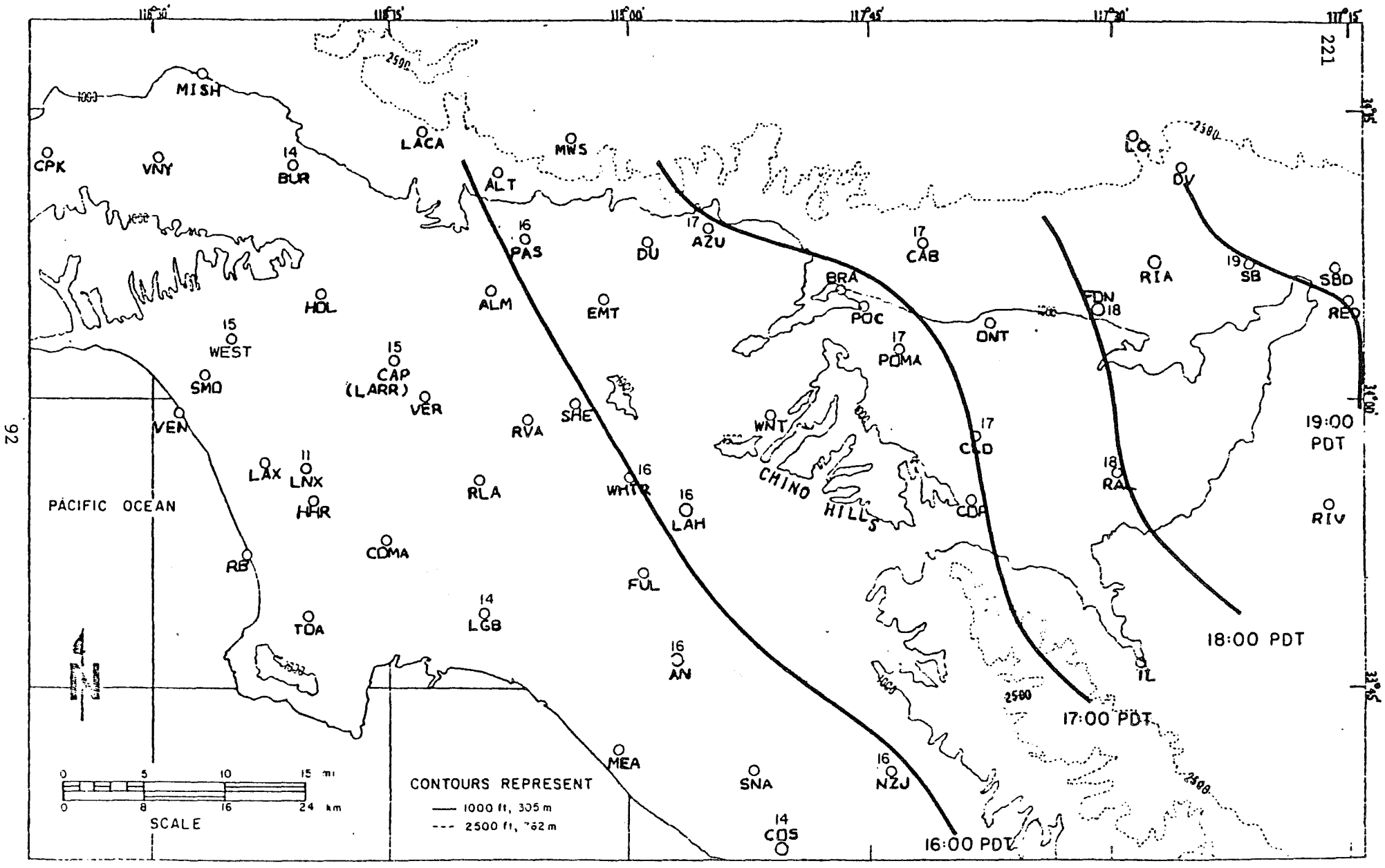


Figure 14. APPROXIMATE TIME (PDT) OF ARRIVAL OF SEA BREEZE, JULY 25, 1973
(Objective criterion based on ground level ozone concentrations.)

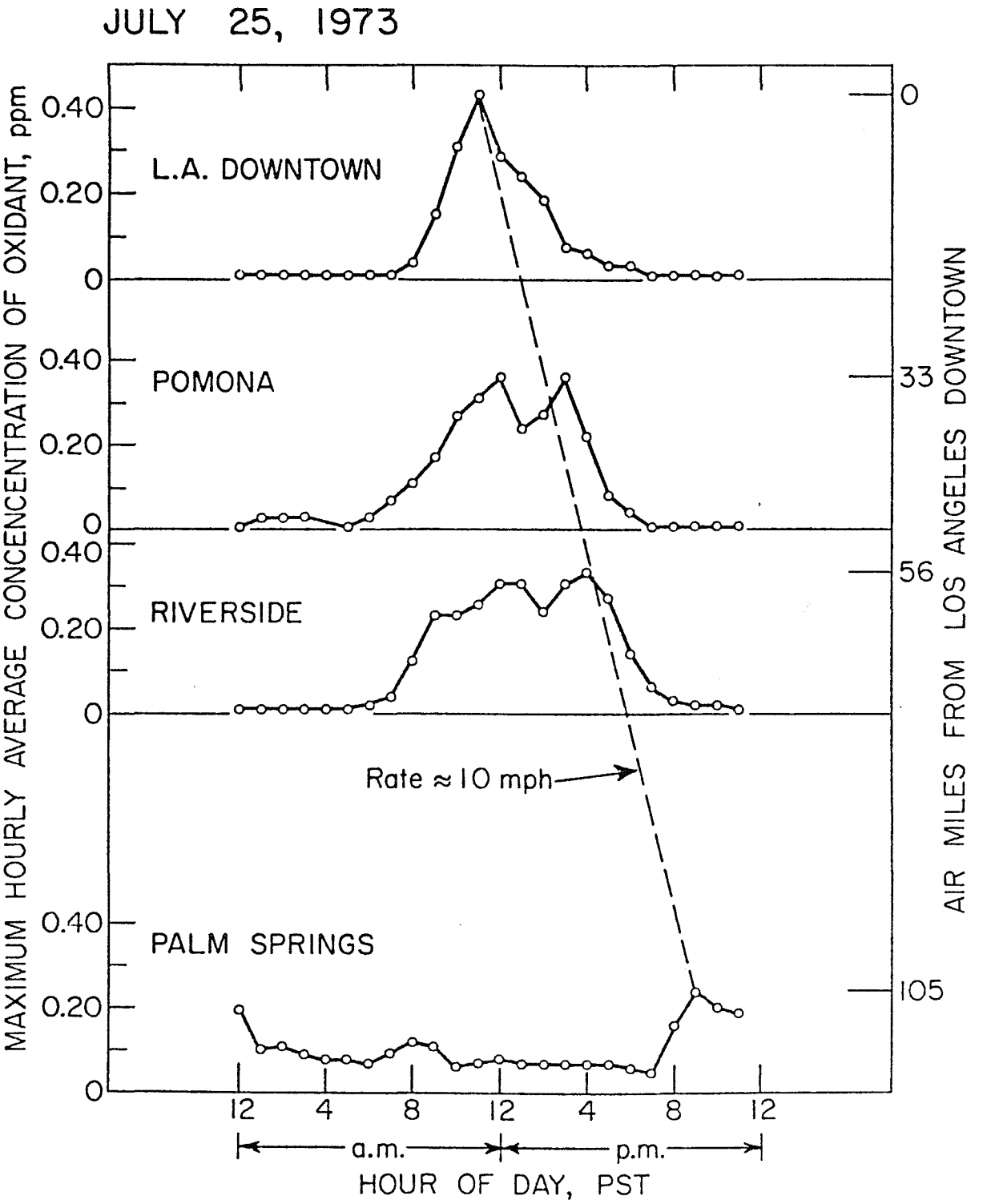


Figure 17. Diurnal variation July 25, 1973, of oxidant concentrations at air monitoring stations at Los Angeles Downtown, Pomona, Riverside, and Palm Springs, California. Values are corrected data: Los Angeles Downtown and Pomona x 1.1 and Riverside and Palm Springs x 0.8.

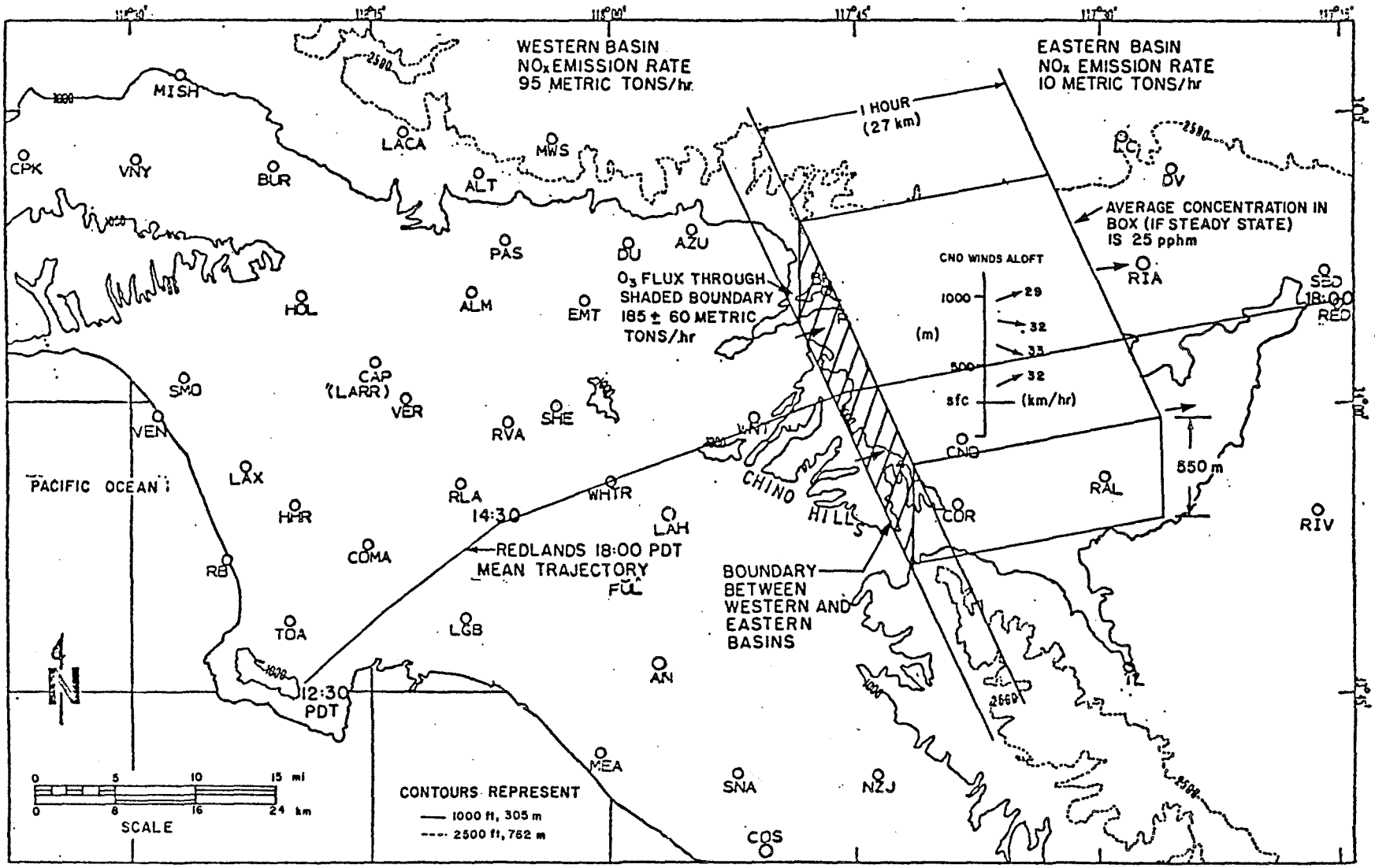


Fig. II-15. ESTIMATED OZONE FLUX FROM WESTERN TO EASTERN BASIN, JULY 25, 1973 1700 PDT

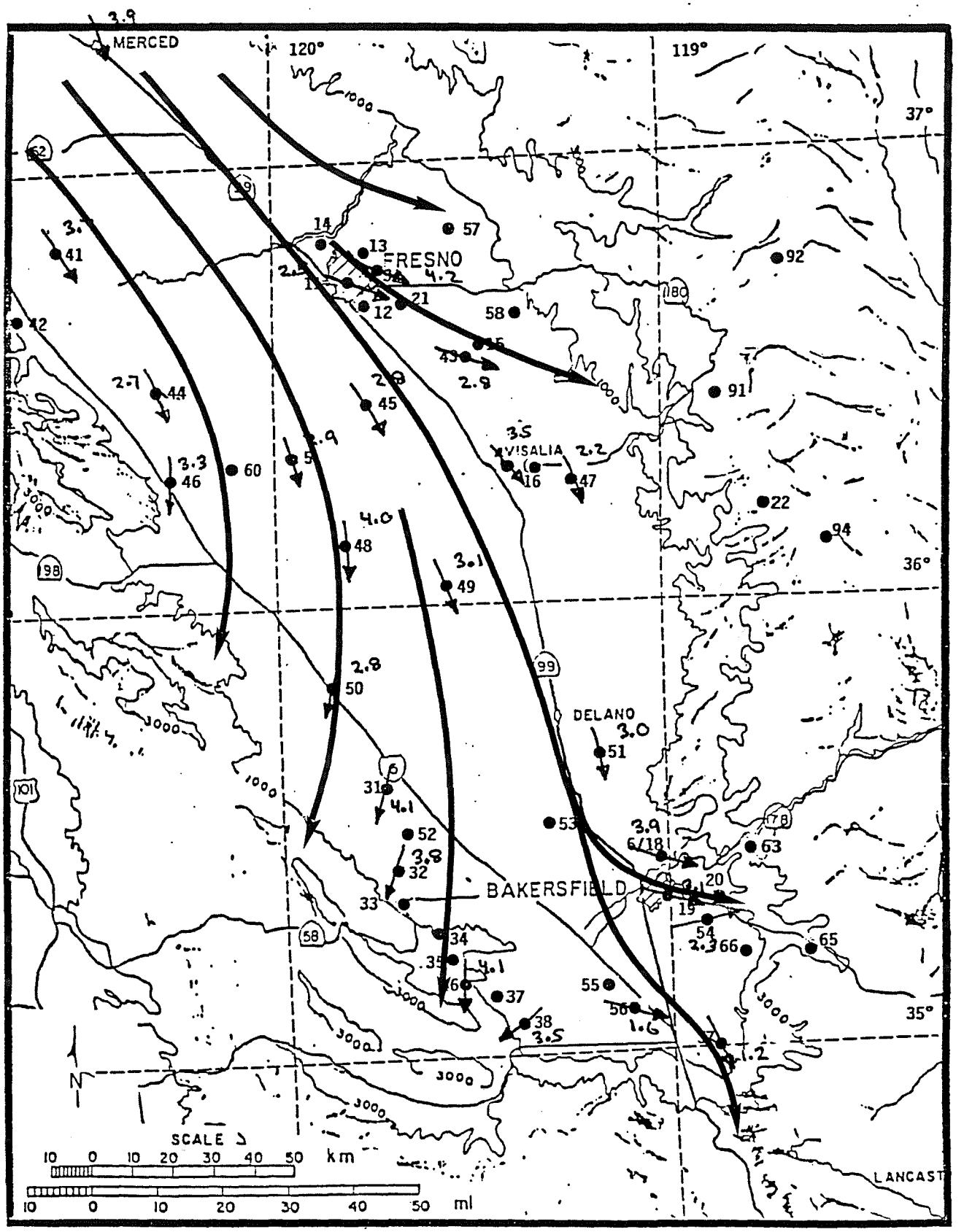


Figure 4-1. Surface streamlines from most frequent wind directions and average wind speeds for those directions for the hours 1500-1700 PDT during the period from 16 July through 17 August 1984. Wind speeds in m/s.

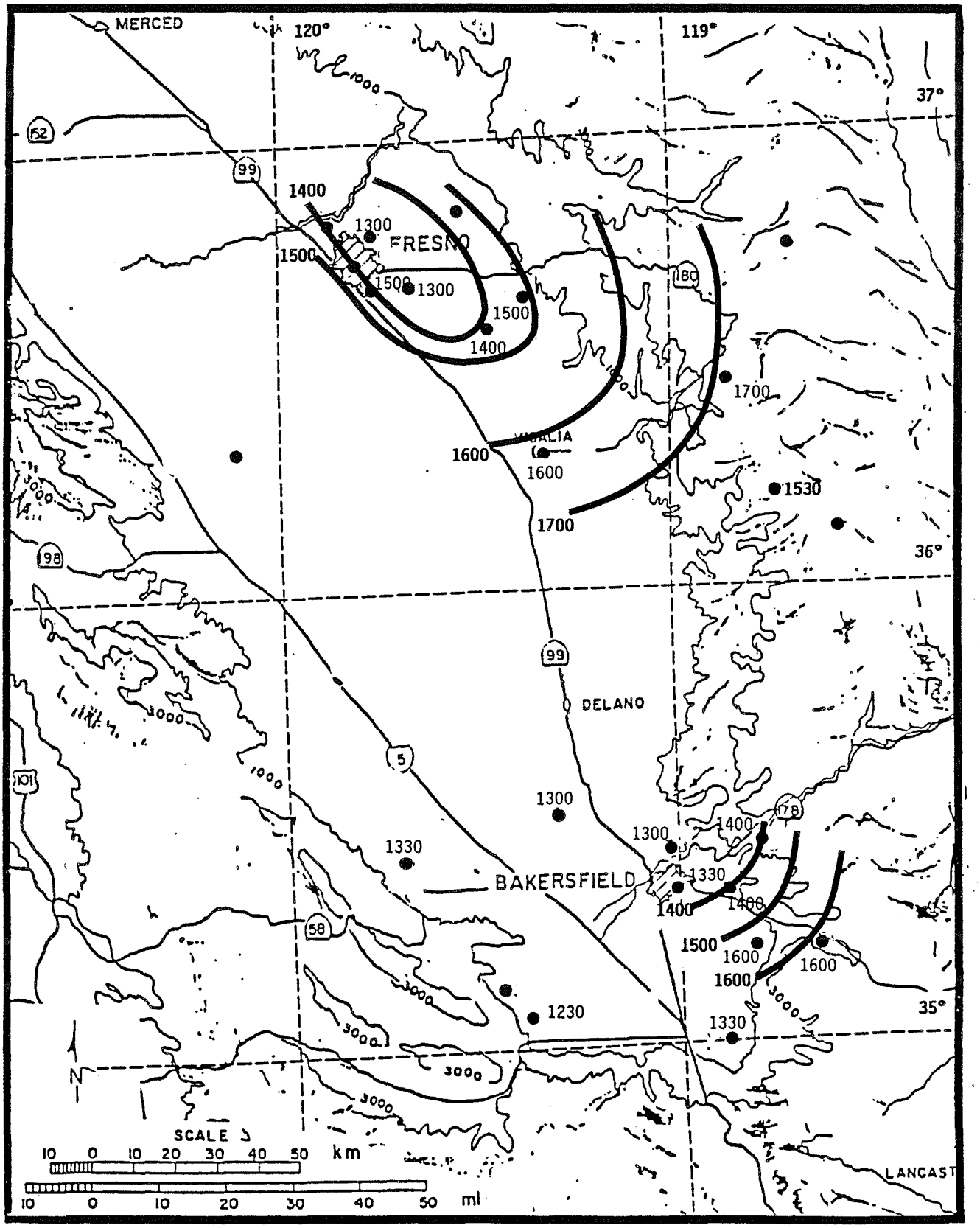


Figure 3-11. Map of median hour of arrival of the peak O_3 concentration for all days in study period with maxima > 10 pphm. (Times shown next to site numbers are PDT.)

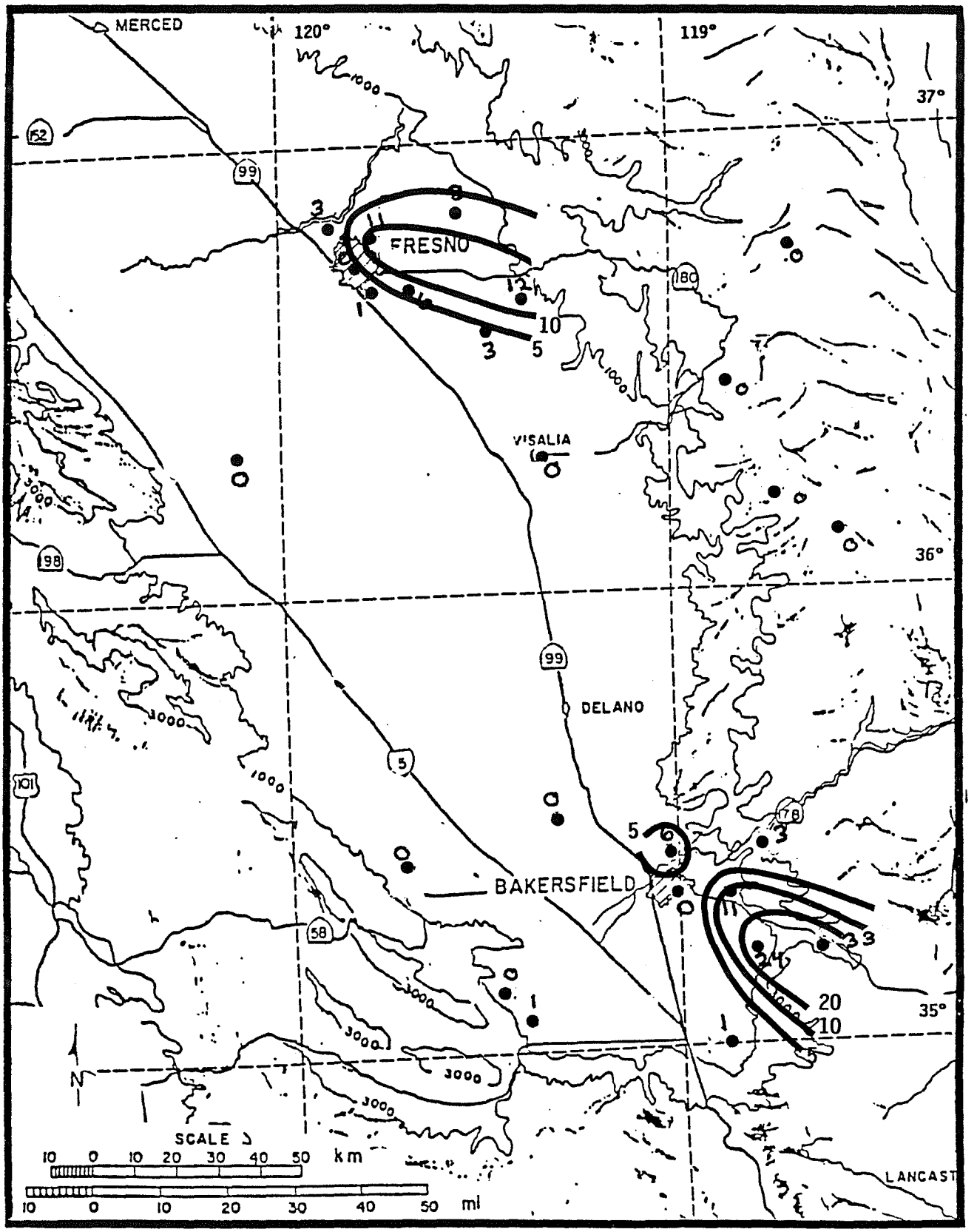


Figure 3-7. Map of the number of hourly average ozone values exceeding 12 pphm from July 15 to August 18, 1985.

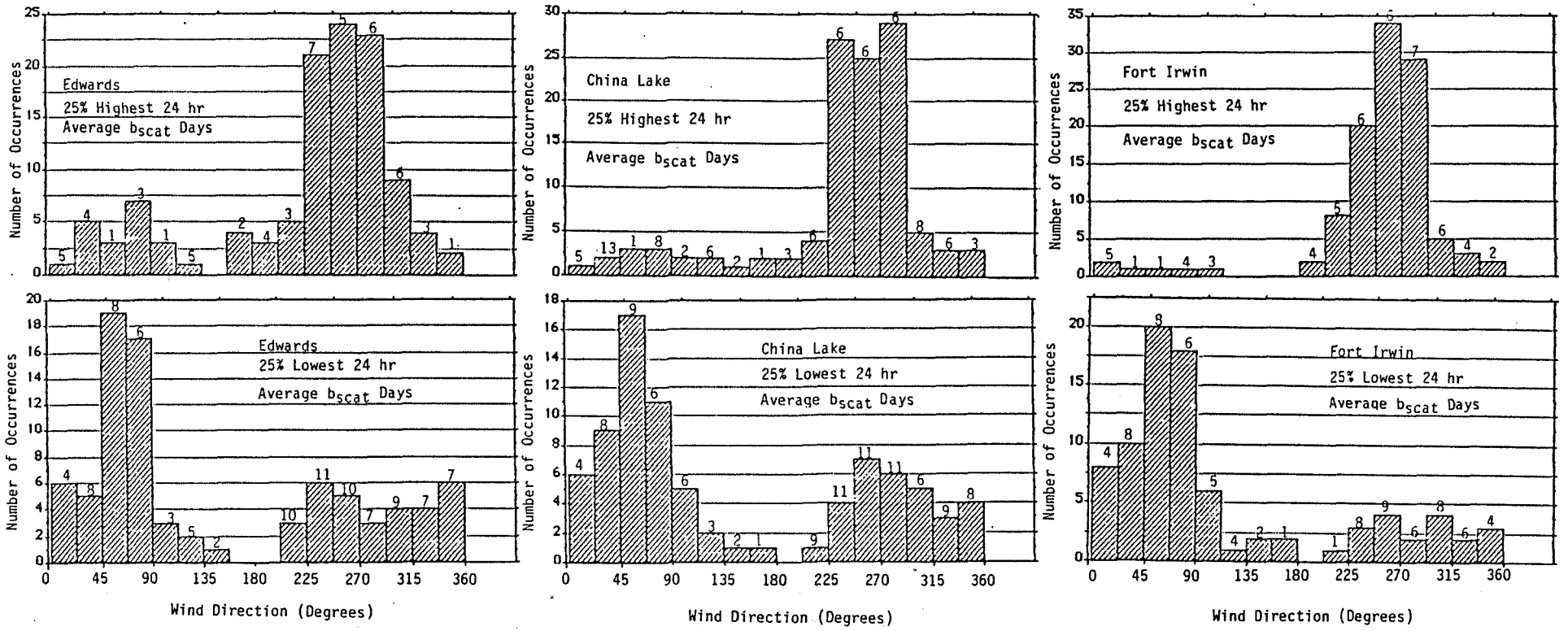


Figure 4-25. Frequency distribution of 850 mb wind directions and average speeds for each direction for A.M. (0000-1200 PST) soundings at Edwards AFB for the 25% highest and 25% lowest 24 hr average b_{scat} days at Edwards, China Lake, and Fort Irwin for August 1983 - July 1985 time period.

Presentation Material

for

Ozone Episode Representativeness Study for the South Coast Air Basin

Prepared for:

ARB/Caltech Conference on Photochemical Modeling as a Tool for Decision Makers
February 1-3, 1988
California Institute of Technology, Pasadena, California

Prepared by:

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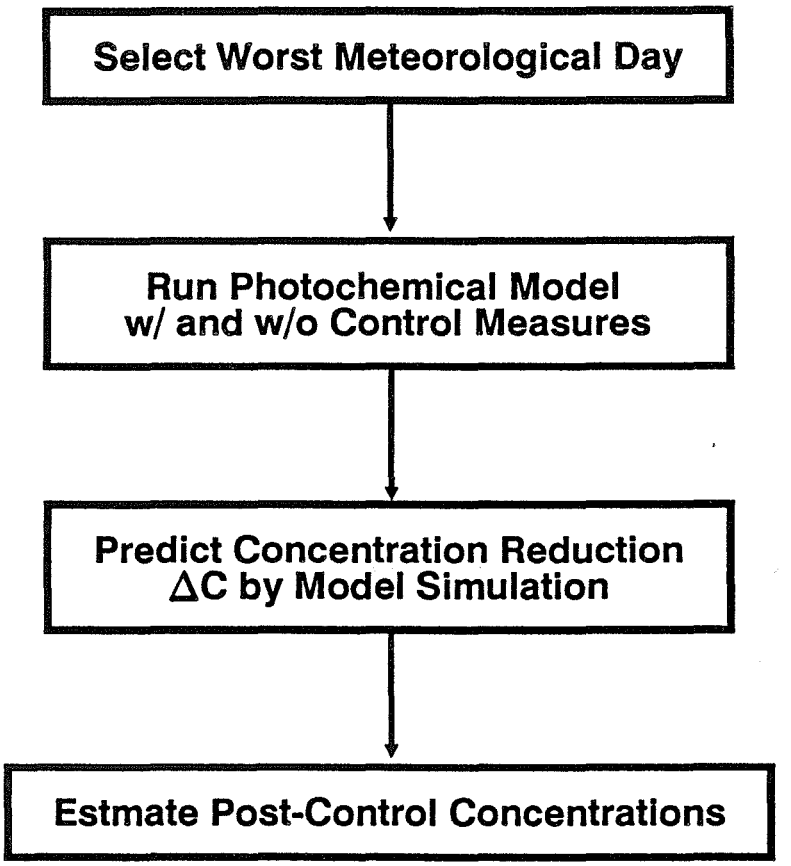
Valley Research Corporation
15904 Strathern Street, Suite 22
Van Nuys, California 91406
(818) 902-0022

Conventional Method for Estimating Post-Control Concentrations



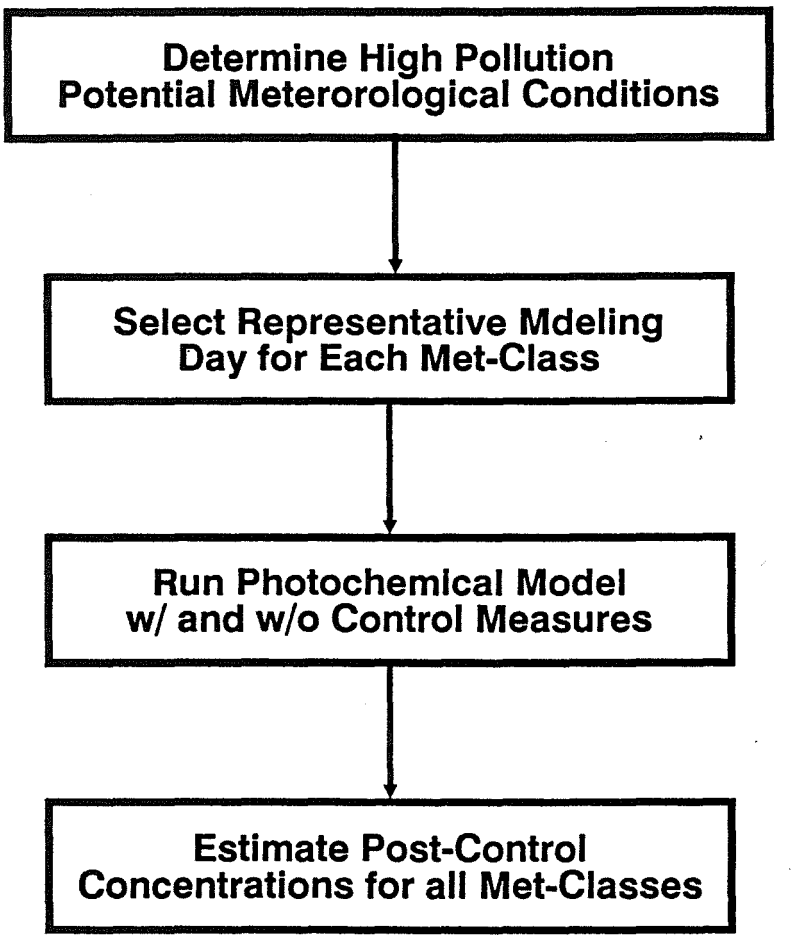
For the i-th Non-Modeling Day

$$C_{post,i} = C_{pre,i} - \Delta C_{model}$$

or

$$C_{post,i} = C_{pre,i} (C_{post}/C_{pre})_{model}$$

New Proposed Method for Estimating Post-Control Concentrations



For the i-th Non-Modeling Day in Met-Class J

$$(C_{ij})_{post} = (C_j)_{pre} - (\Delta C_j)_{model} + s_j N_i(0,1)$$

where

C_j = mean pre-control concentration of Met-Class J

s_j = standard deviation of concentrations in Met-Class J

$N_j(0,1)$ = a random number drawn from a STD Normal Dist.

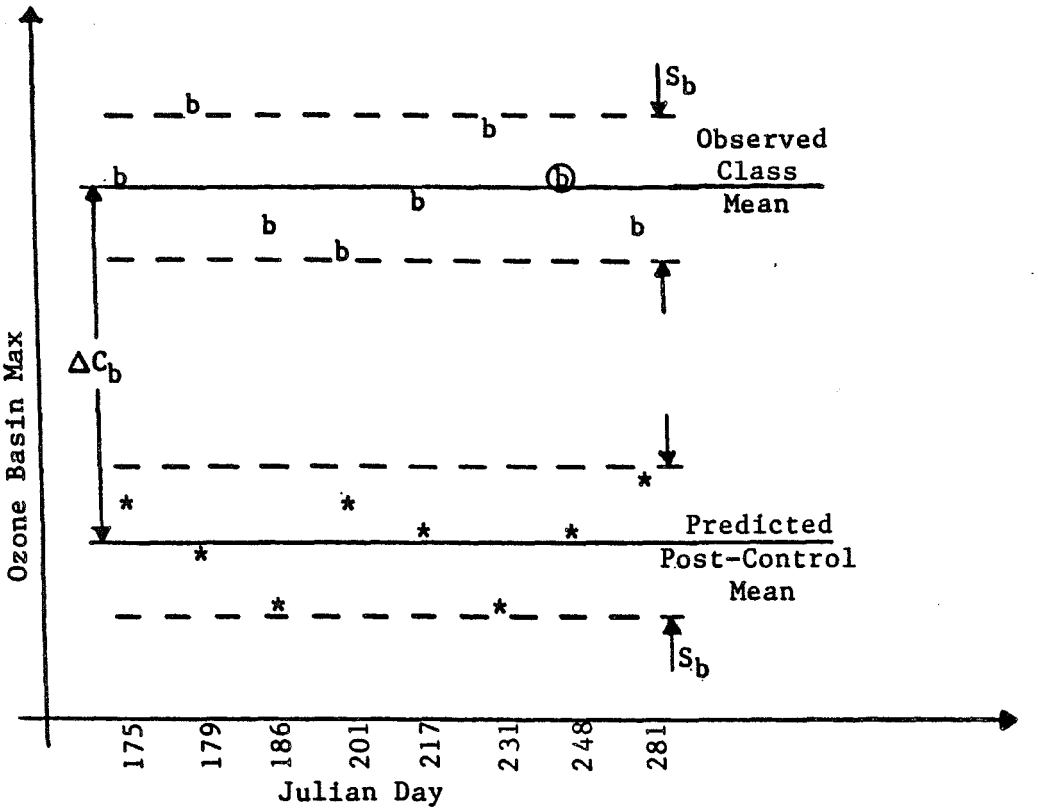


Figure 4-2. Methodology for Predicing Distribution with Control Measures in Place.

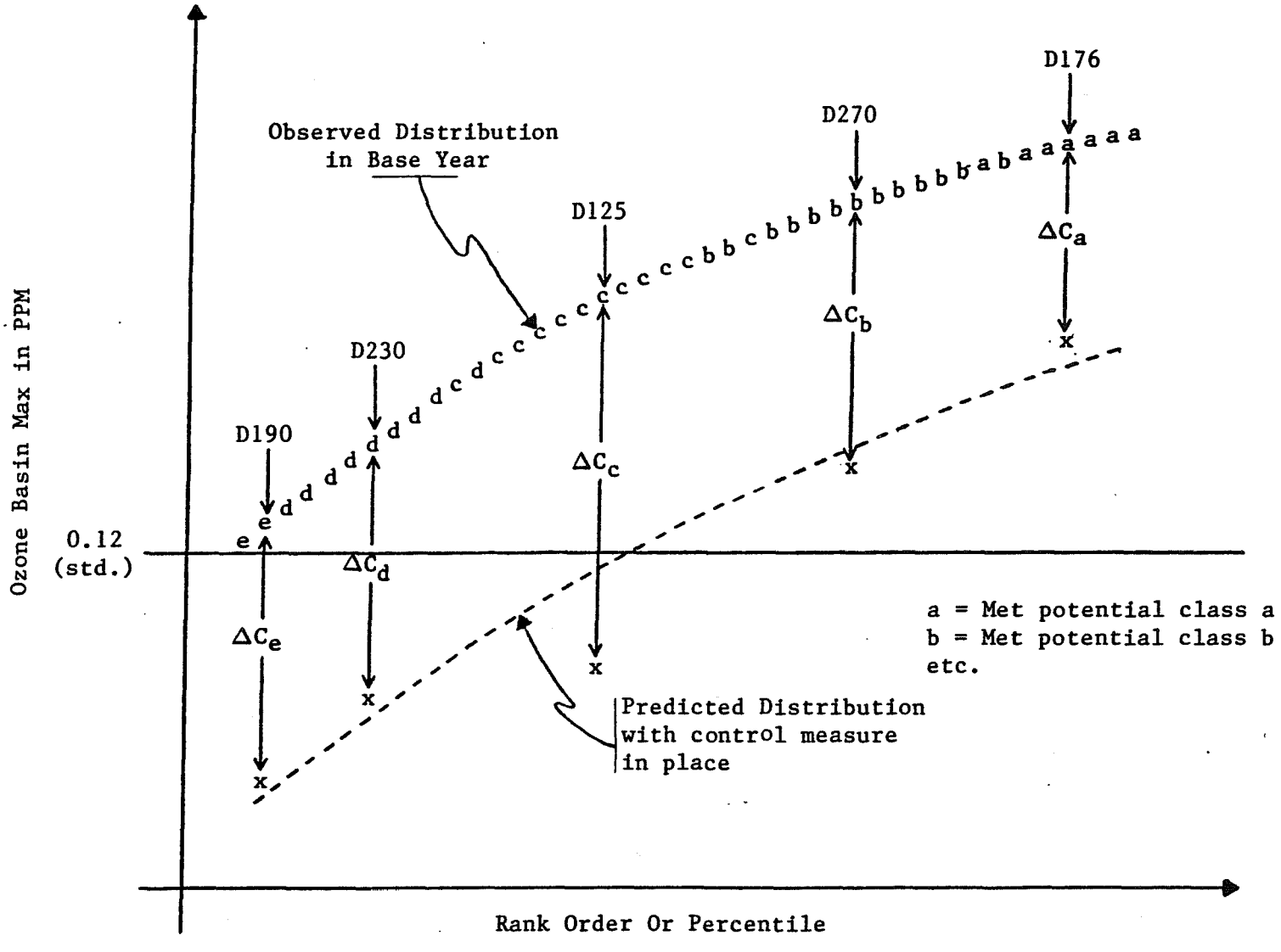


Figure 4-1. Upper Tail Distributions of Base Year Ozone Concentrations and Predicted Concentrations with Control Measures in Place.

CART DECISION TREE

Cart successively partitions the data set into two most dissimilar groups to reduce the sum of variances and then trim marginal branches to obtain the optimal size tree.

Splitting Rule

$$\underset{S_j \epsilon S_J}{MAX}\ RSS_b = RSS_o - RSS_1 - RSS_2$$

where

RSS_o = residual sum of the squares for all cases in the data set,

RSS_1, RSS_2 = residual sum of the squares within each group (in this study, meteorological class),

RSS_b = residual sum of the squares between the two groups, and

S_j, S_J = optimal split on j-th variable and optimal splits for J variables.

Termination Rule

$$\underset{T}{MIN}\ R_a(T) = R(T) + aT$$

where

$R(T)$ = percent of the variance unexplained by the tree with T terminal nodes,

a = cost of penalty imposed on the complexity of a tree, and

$R_a(T)$ = overall cost associated with the tree of T terminal nodes and complexity parameter a.

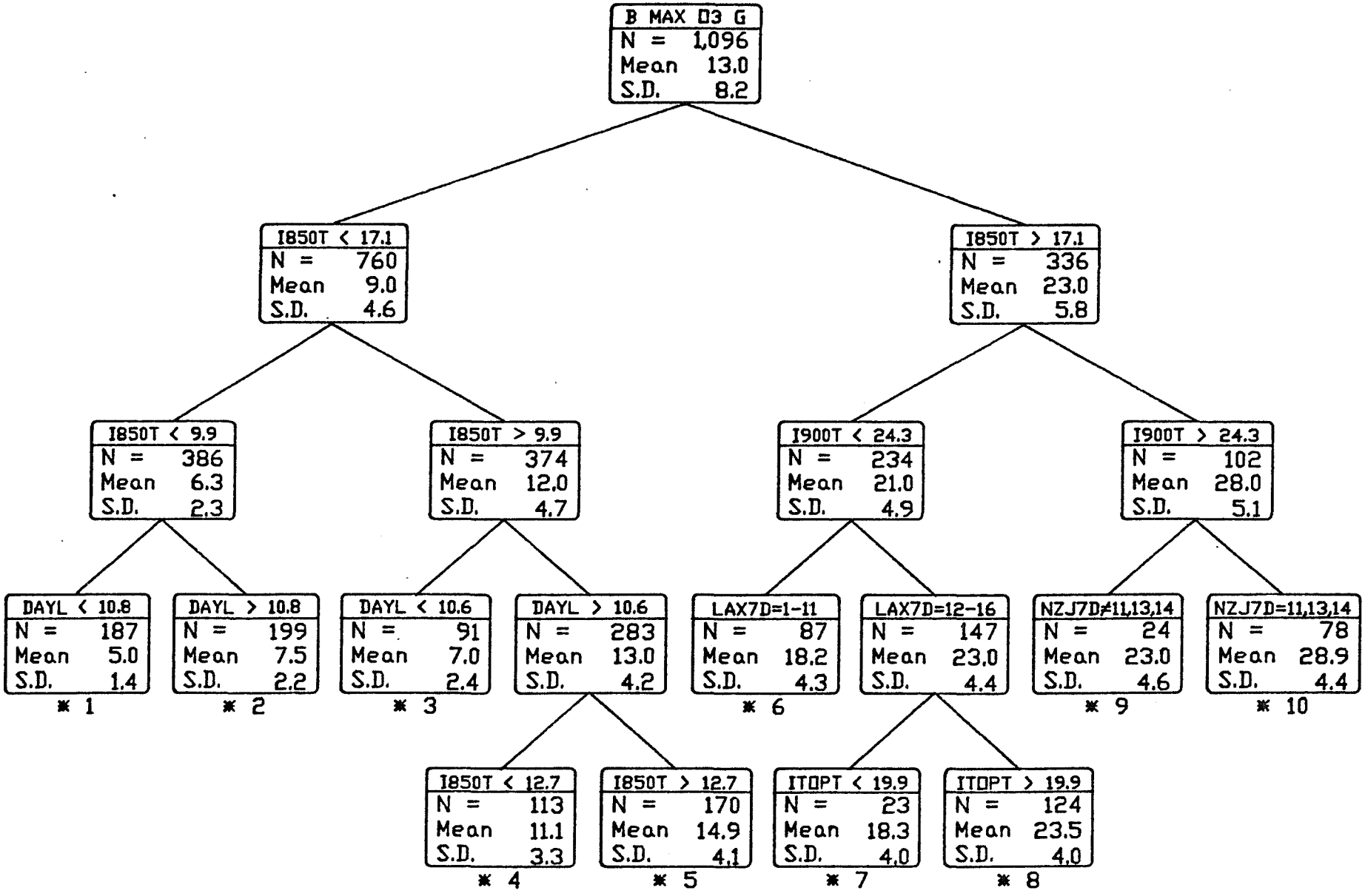
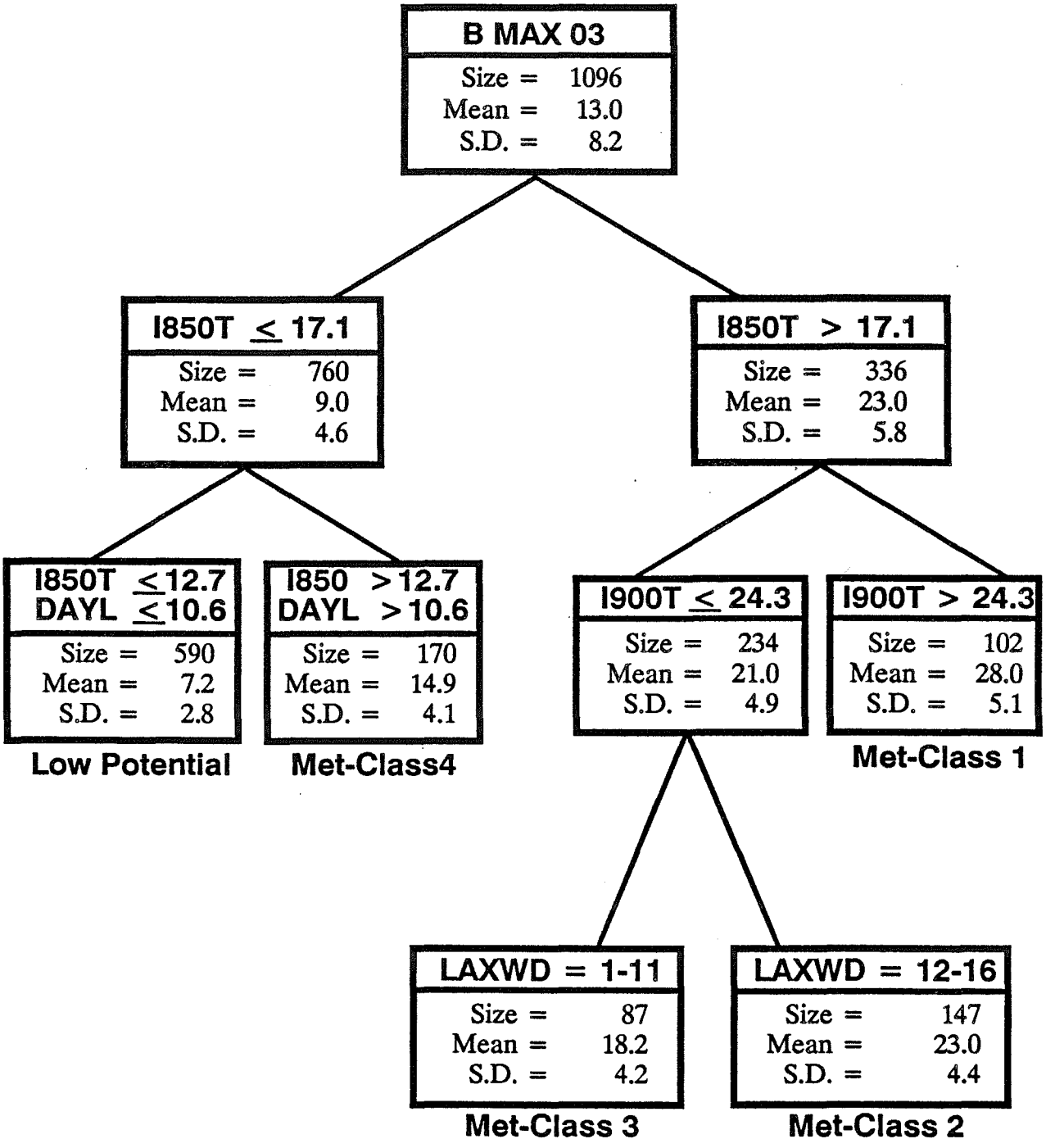


Figure 2-2. Decision Tree For Daily Basin Maximum Ozone Concentrations (Including those measured at Glendora)

CART Generated Met-Classes



PVE = 80

r = 0.9

MEASURE OF DAY'S CENTRAL TENDENCY

The smaller the day's deviation index, the better the day's representativeness for the met-class.

Deviation Index (DI) for the ith Day

$$DI_i = \underset{k}{SUM}\ RI_k \left| X_{ik} - \bar{X}_k \right| / S_k$$

where

RI_k = Relative importance of the k-th variable for explaining intra-class ozone variation,

X_{ik} = i-th day value of the k-th variable,

$\bar{X}_k$ = class mean of the k-th variable, and

S_k = standard deviation of the k-th variable.

Relative Importance of Variables in Total Set and Each Met-Class

Variable	Total Set	Met-Class 1	Met-Class 2	Met-Class 3	Met-Class 4
INV850T	100	100	0	0	0
INV900T	84	53	15	0	24
INV950T	36	54	10	31	1
INV1000T	30	2	74	48	21
INVBAST	46	2	66	2	27
INVTOPT	75	0	0	0	30
HT500	63	64	0	0	6
SANLAS	13	0	11	32	12
SUM15Z	19	37	5	12	29
LAX7CWD	34	0	3	64	65
LAX13CWD	18	0	0	41	60
LAX13RWS	19	0	45	100	25
LAX13WF	15	13	0	98	23
NZJ7CWD	41	0	0	59	43
NZJ13CWD	24	0	0	8	100
LGB13CWD	15	0	10	0	34
RIV7CWD	27	0	43	56	47
DAYLNGTH	71	0	0	13	14

Mean Ozone Concentrations on Days in Each Met-Class and on Two Preceding Days

Met-Class		Ozone Levels in PPHM		
		Day-2	Day-1	Day
1	Mean	24.4	27.4	28.4
	S.D.	6.2	5.1	4.4
2	Mean	21.3	22.1	23.5
	S.D.	5.6	4.3	4.0
3	Mean	21.6	20.4	18.2
	S.D.	6.1	5.8	4.3
4	Mean	13.7	14.4	14.9
	S.D.	6.1	4.6	4.1

Candidate Modeling Days for Four Met-Classes

Met-Class	Candidate Day	Day of Week	Rank in Met-Class	Basin Max Ozone D-2	D-1	D
1	8/27/83	Sat	2nd	24	32	33
1	8/28/85	Wed	8th	18	26	30
2	8/03/84	Fri	5th	20	20	27
3	7/06/85	Sat	3rd	23	21	22
3	7/28/83	Thurs	9th	19	16	17
4	6/21/84	Thurs	3rd	16	15	16
4	10/05/84	Fri	7th	12	13	13
4	10/30/85	Wed	8th	11	14	13
4	3/10/84	Sat	12th	13	13	15

Rating of Presently Used Modeling Days

Met-Class	Modeling Day	Day of Week	Rank in Met-Class	Basin Max Ozone D-2	D-1	D
1	6/27/74	Thurs	62nd	34	34	46
2	8/30/82	Mon	57th	15	17	18
2	8/31/82	Tues	28th	17	18	26
1	9/01/82	Wed	40th	18	26	35
1	9/02/82	Thurs	79th	26	35	40
2	8/07/84	Tues	9th	22	32	29
1	8/08/84	Wed	58th	32	29	31

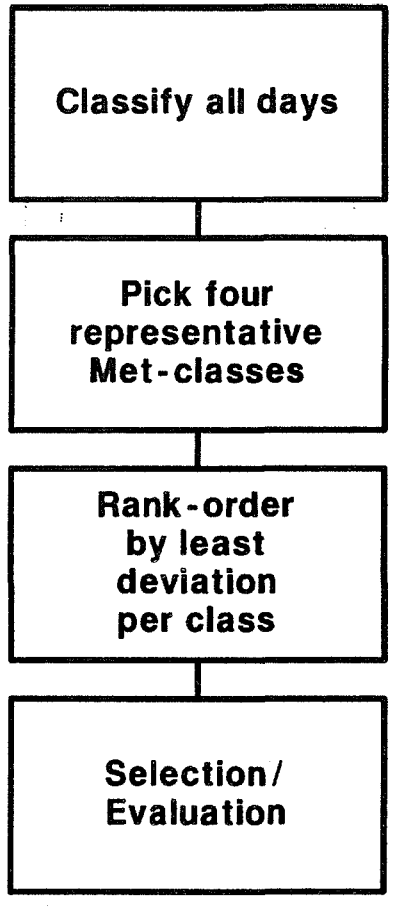
Ozone Episode Representativeness Study:

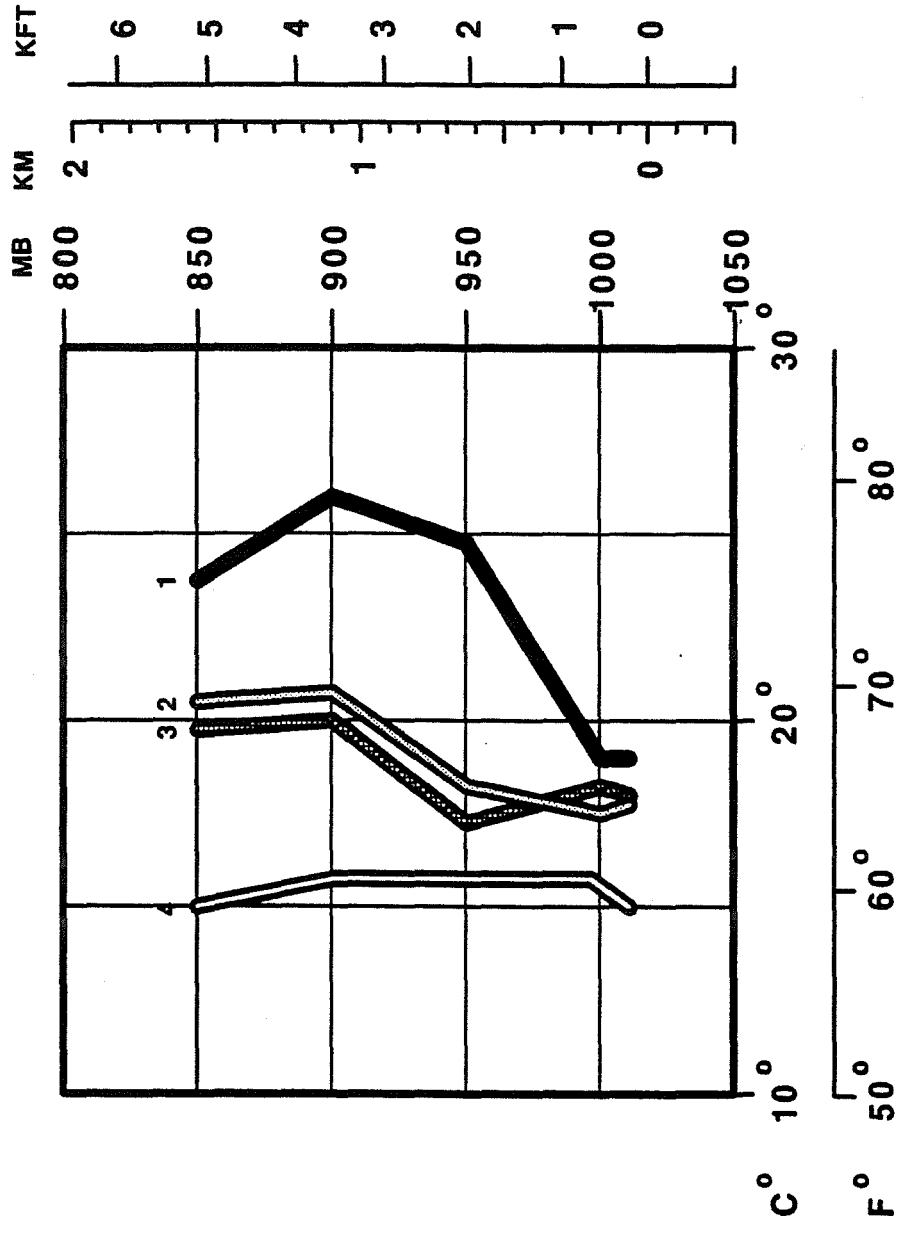
A Critique of Y. Horie's Procedures

M. Zeldin

Southern California Edison

General Methodology



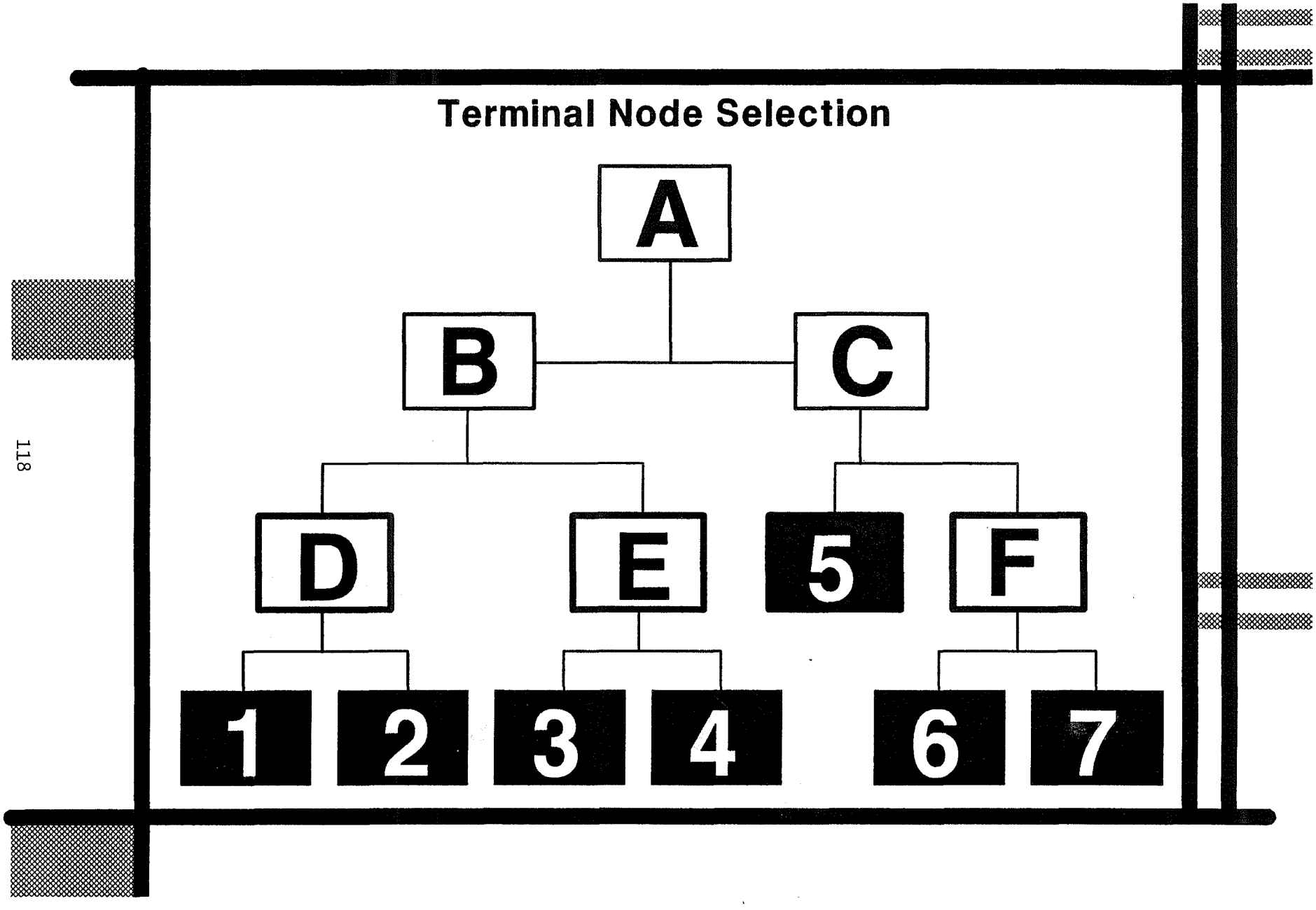

KFT
6
5
4
3
2
1
0
KM
2
1
0
MB
800
850
900
950
1000
1050
30°
20°
10°
C°
80°
70°
60°
50°
F°
1
2
3
4

Strengths

- Objective method
- Uses good selection of meteorological variables
- Can evaluate individual days

Suggested Improvements

- Seasonality
- Week-end exclusion
- Terminal node selection
- Distributions by Met-class
  - "DI" factor for ozone
  - Multi-day sequence of Met-classes


Terminal Node Selection
A
B
C
D
E
5
F
1
2
3
4
6
7

Suggested "Deviation Index"

$$A\,(\text{Met DI}) + B\,(O_3\ \text{DI})$$

where $A = 0.7$, $B = 0.3$

if $O_3\ \text{DI} < 1.00$

else $A = 0.3$, $B = 0.7$

and $$O_3\ \text{DI} = \frac{X_i - \bar{X}}{S_x}$$

Frequency of Class Sequence

(Example)

	5 → 1	4 → 1	3 → 1	2 → 1	1 → 1
①	3	10	25	**81**	32

	5 → 3	4 → 3	3 → 3	2 → 3	1 → 3
②	27	**41**	21	**35**	32

Summary

- CART — use appropriate data
  - use 4 inclusive nodes
- DI — include ozone
- Multi-Day Sequencing
- ⇨ — should result in about 6 modeling days which represent about 80% of all summer days

Episode Selection To Meet Regulatory Needs

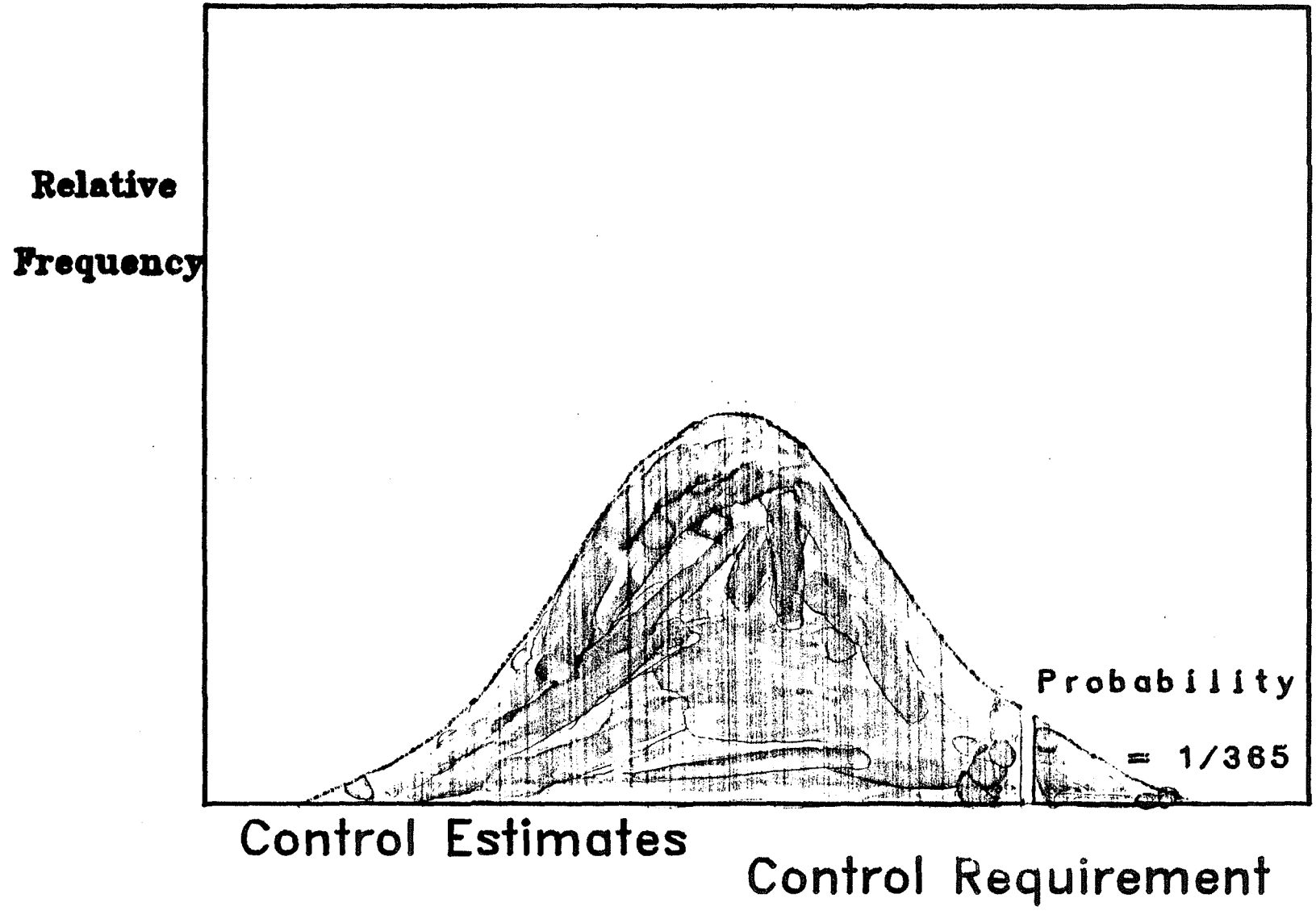
* *NAAQS & CAA Requirements*
* *Historical Perspective Using EKMA and Airshed*
* *Ideas for Airshed/Post-'87 SIP's*

K. GOLDEN
U.S. ENVIRONMENTAL PROTECTION AGENCY

OZONE NAAQS

The NAAQS for ozone is attained when the expected number of days per calendar year with maximum hourly average concentrations above 0.12 ppm is one or less.

Control Requirements Needed To Demonstrate Attainment Of Ozone NAAQS



DEFINITIONS

Design Day = *Modeling episode used to estimate SIP Control requirement necessary to achieve the NAAQS.*

Monitored Design Value = *4th highest ozone concentration observed at a site during a 3 year period.*

Achievement of NAAQS depends on :

- Observed & Predicted Maximum O_3 Values
- Transported Ozone
- NMOC/NOx ratio
- Atmospheric dilution
- Differing patterns of fresh emissions

Example Calculation Of Design Day Using EKMA

O_3	Date	% Reduction
.22	6/8/87	58
.19	8/25/86	51
.19	10/2/86	54
.18	8/26/86	52
.17	7/26/85	49

Ventura County
Identification Of Transport Days
Fourth Highest Values And Design Day
1982–1984 Air Quality Data

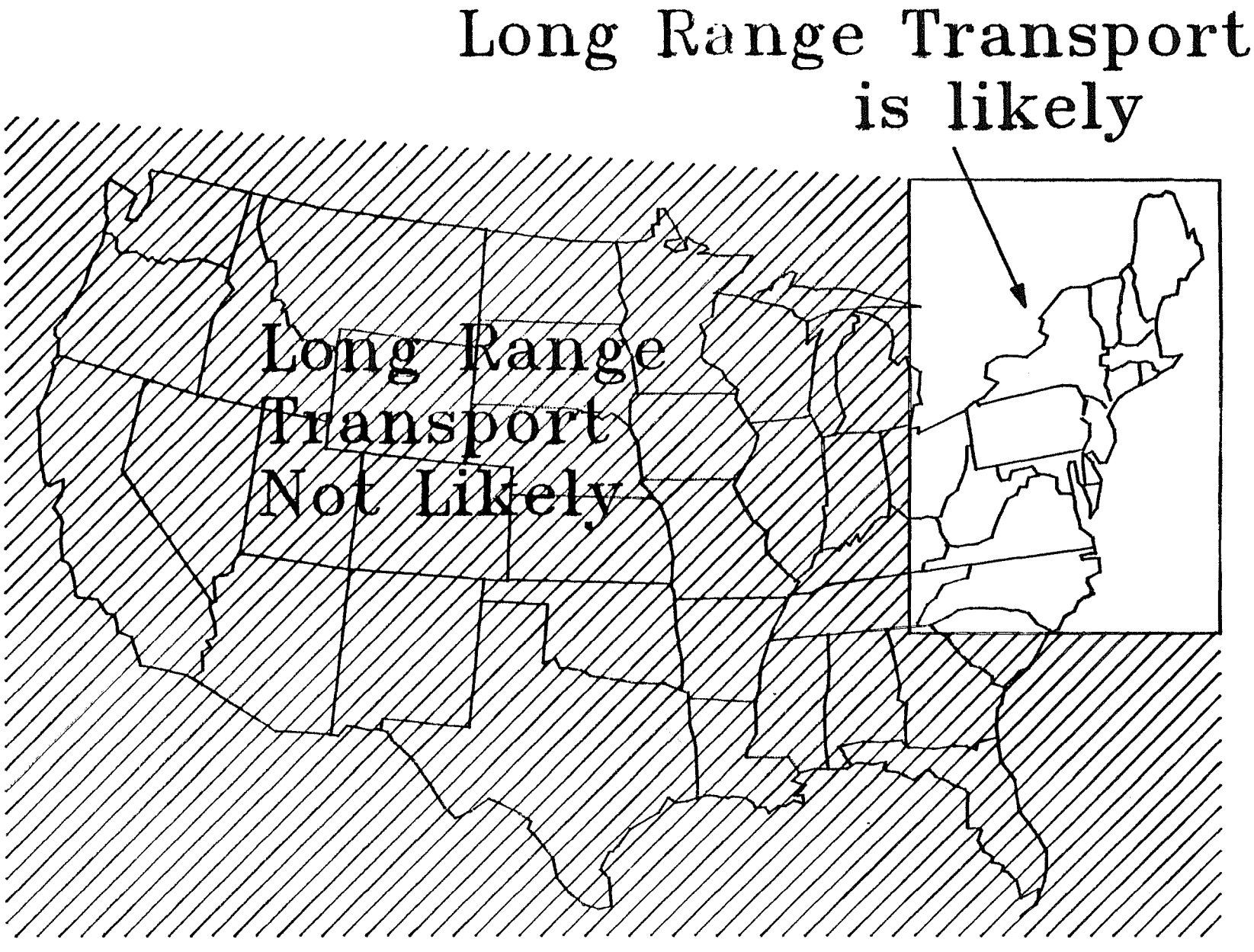
Station	Date	(ppm) Value	Transport	Fourth Highest	Design Day
Ojai	7–23–82	0.16		*	
	8–22–82	0.16		*	
	5–19–83	0.17			
	7–14–83	0.17			
	8–07–82	0.18			
Simi Valley	7–12–82	0.17		*	
	7–15–82	0.17		*	
	7–21–82	0.17		*	
	8–01–82	0.17		*	
	9–17–83	0.17		*	*
	7–31–82	0.18	*		
	8–07–82	0.18	*		
	8–23–82	0.18	*		
	10–19–83	0.18	*		
	8–09–84	0.19	*		
	10–20–83	0.21	*		
	7–30–82	0.22	*		
	8–06–82	0.23	*		
	9–12–83	0.23	*		

Ventura County
Identification Of Transport Days
Fourth Highest Values And Design Day
1982–1984 Air Quality Data

Station	Date	(ppm) Value	Transport	Fourth Highest	Design Day
Ventura	4–23–82	0.16		*	
	8–06–83	0.16		*	
	10–27–83	0.17			
	9–28–84	0.17			
	9–29–84	0.19			

Criteria Used To Link 1980 Episodes to Design Day Selection

1) Surface Winds
2) Upper Level Winds
3) Diurnal O_3
4) Inversion Strength
5) Maximum Surface Temperature


Long Range Transport is likely
Long Range Transport Not Likely

Design Day As A Function Of Incidents Of Overwhelming Transport*

Number of Transport Cases	Design Day Candidate
0	Fourth highest monitored O_3 value
1	Third highest monitored O_3 value
2	Second highest monitored O_3 value
≥ 3	Highest monitored O_3 value

* Table assumes all sites have 3 years of valid data. For selecting "SIP Design Day" additional factors must also be considered.

Design Day Selection Using Multiple Airshed Simulations

1) Calculate monitored design value (MDV).

2) Identify candidate modeling days based upon MDV value ($\pm$ 20%) and Meteorology groupings.

3) Perform Airshed simulations for perhaps 5 episodes.

4) "Rank" Airshed simulations according to emission reduction estimate needed to attain the NAAQS, and frequency of occurance of meteorology class/monitored ozone value.

C. LIU
SOUTH COAST AIR QUALITY
MANAGEMENT DISTRICT

QUESTION :

Why the results of Urban Airshed Model applications were not effectively incorporated in ozone air quality planning in the South Coast Air Basin?

EXPECTATION

- Attainment Demonstration
- Control Effectiveness Assessment

CASE EXAMPLE

EPISODE : 26 - 27 June 1974

INTENTS:

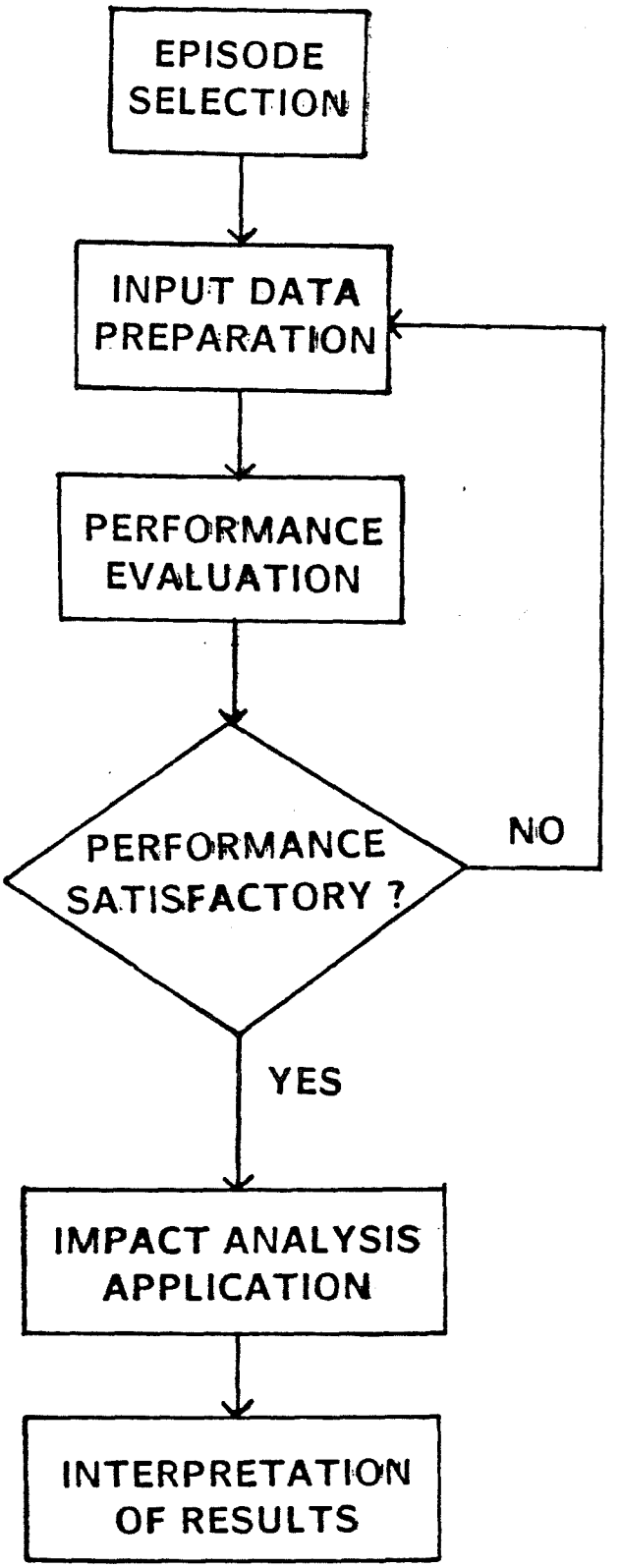
(1) To Demonstrate attainment with 80% ROG Emission Reduction

(2) To Determine the Effect of Emission Controls on Ozone Air Quality

URBAN AIRSHED MODELING SCENARIOS

Scenario	Emission Reduction (%) ROG	NOx
1987 Base Case	0	0
Control for ROG Only to Meet Ozone Standard	80	0
Control for Both ROG and NOx (AQMP)	25	22

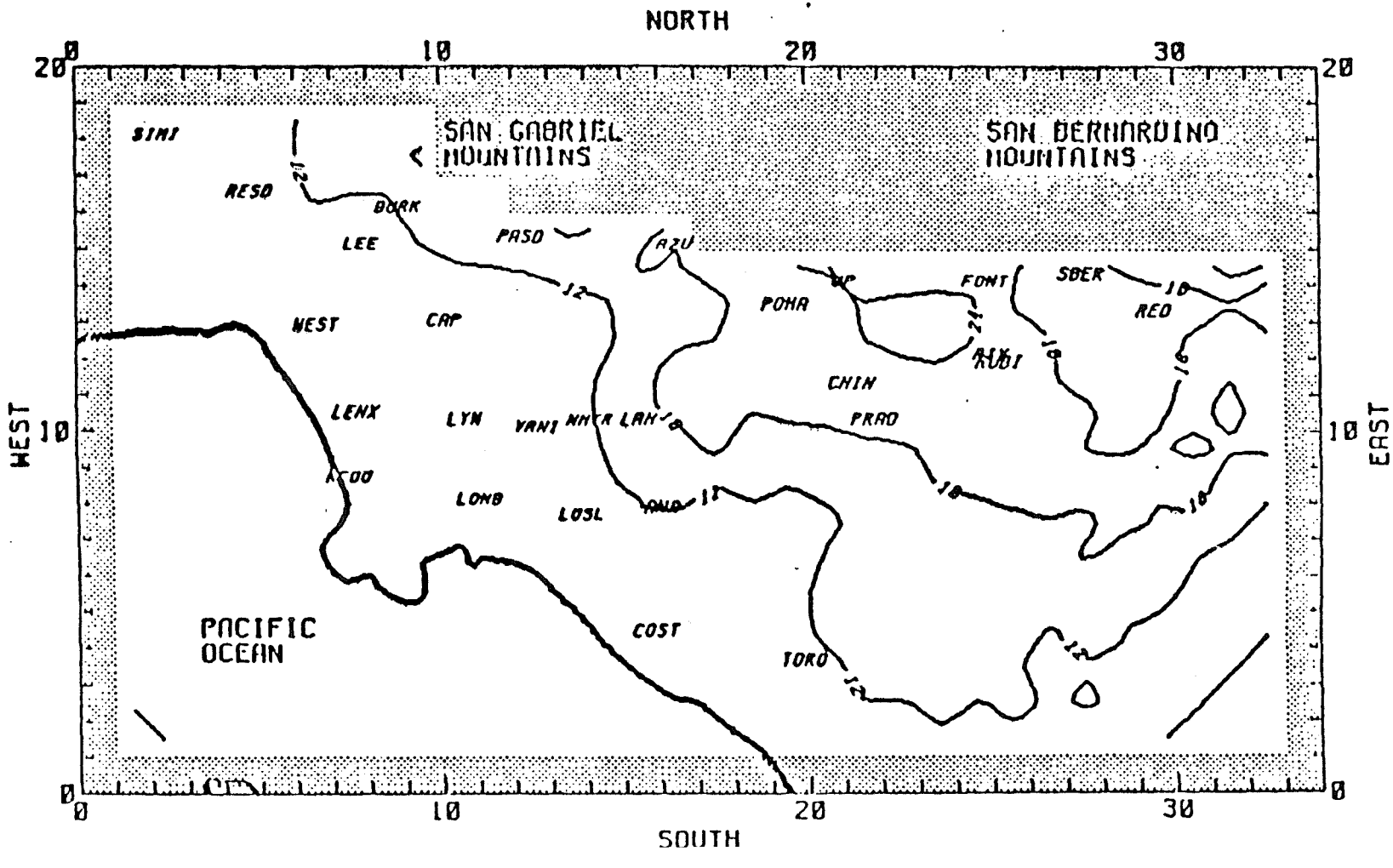
URBAN AIRSHED MODEL APPLICATION FLOW DIAGRAM



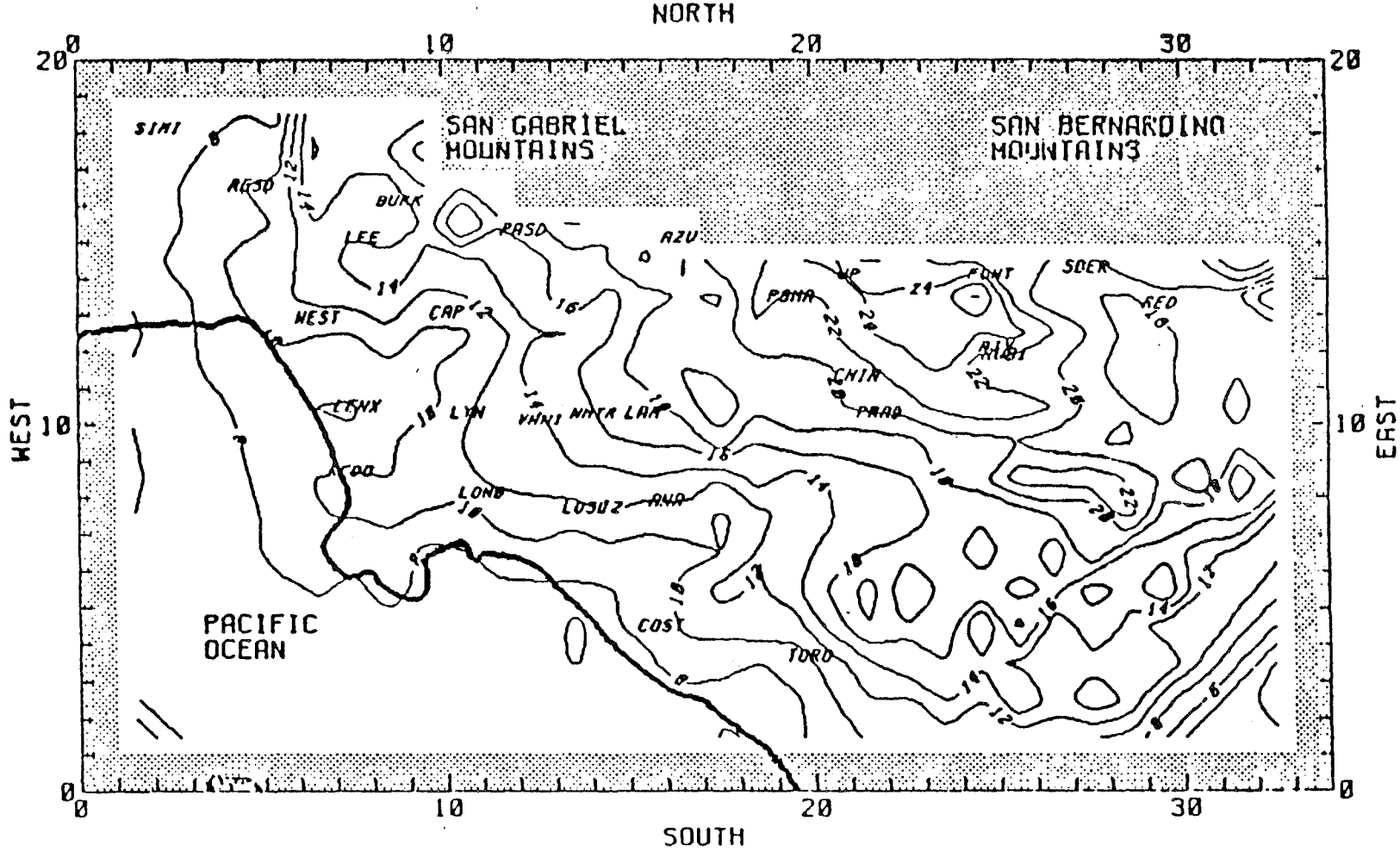
COMPARISON OF PEAK OZONE CONCENTRATIONS

Type	Station	Conc. (pphm)	Hour
Observed Peak Station	Upland	49	1400
Predicted Peak Everywhere	--	39	1600
Predicted Peak Station	Fontana	35	1600
Observed Conc. at Predicted Peak Station	Fontana	48	1500
Predicted Conc. - 1987 Base Case	Fontana	26	1600
Predicted Conc. - 80% ROG Control	Fontana	13	1600
Predicted Conc. - 25% ROG Control & 22% NOx Control	Fontana	24	1600

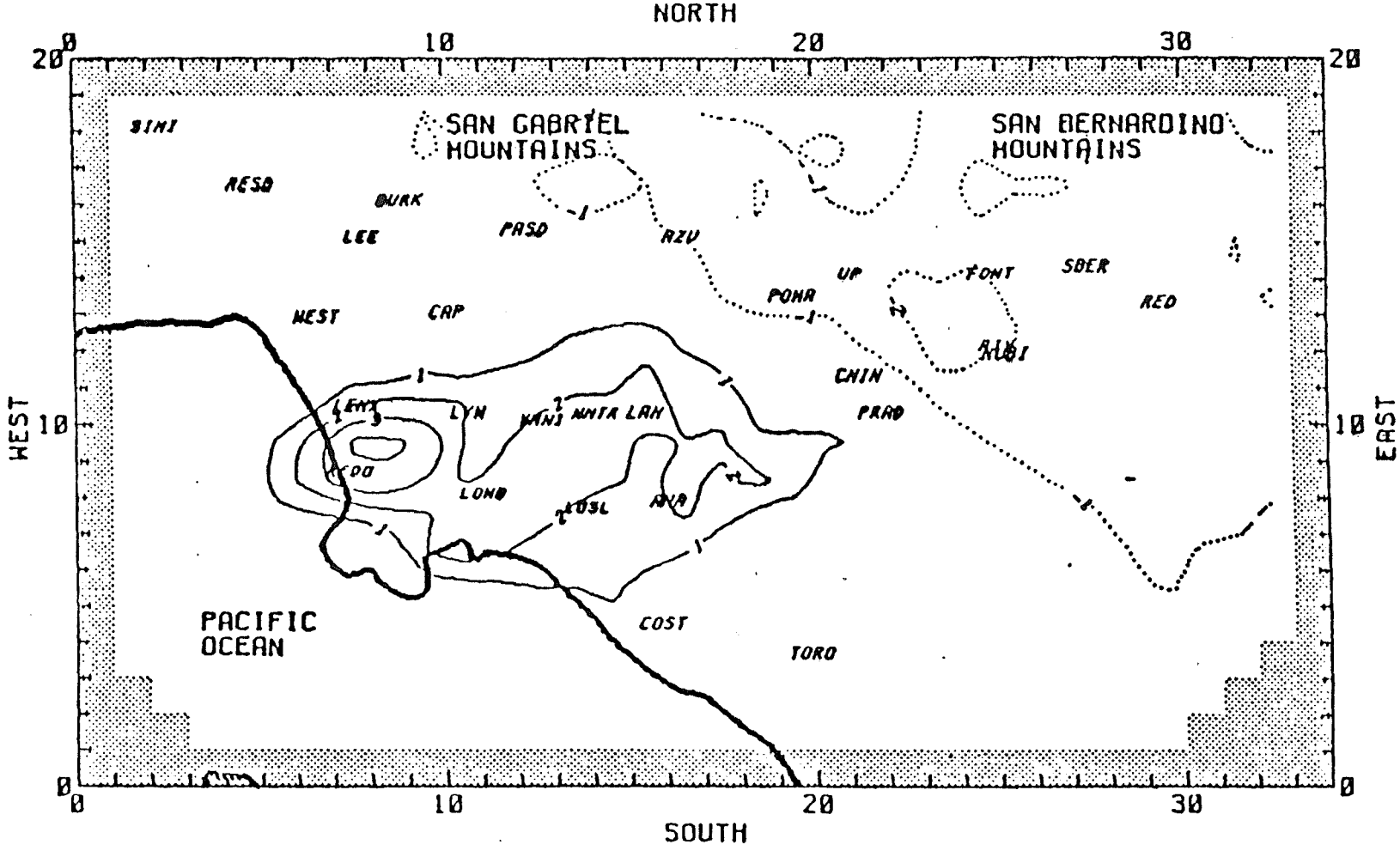
MODEL PREDICTED CONCENTRATIONS (pphm) FOR THE HOUR 1500-1600 (1987 Base Case)



MODEL PREDICTED MAXIMUM CONCENTRATIONS (pphm)
ANY HOUR (1987 Base Case)



CHANGES OF MODEL PREDICTED MAXIMUM OZONE CONCENTRATIONS (pphm) WITH THE IMPLEMENTATION OF AQMP CONTROL MEASURES

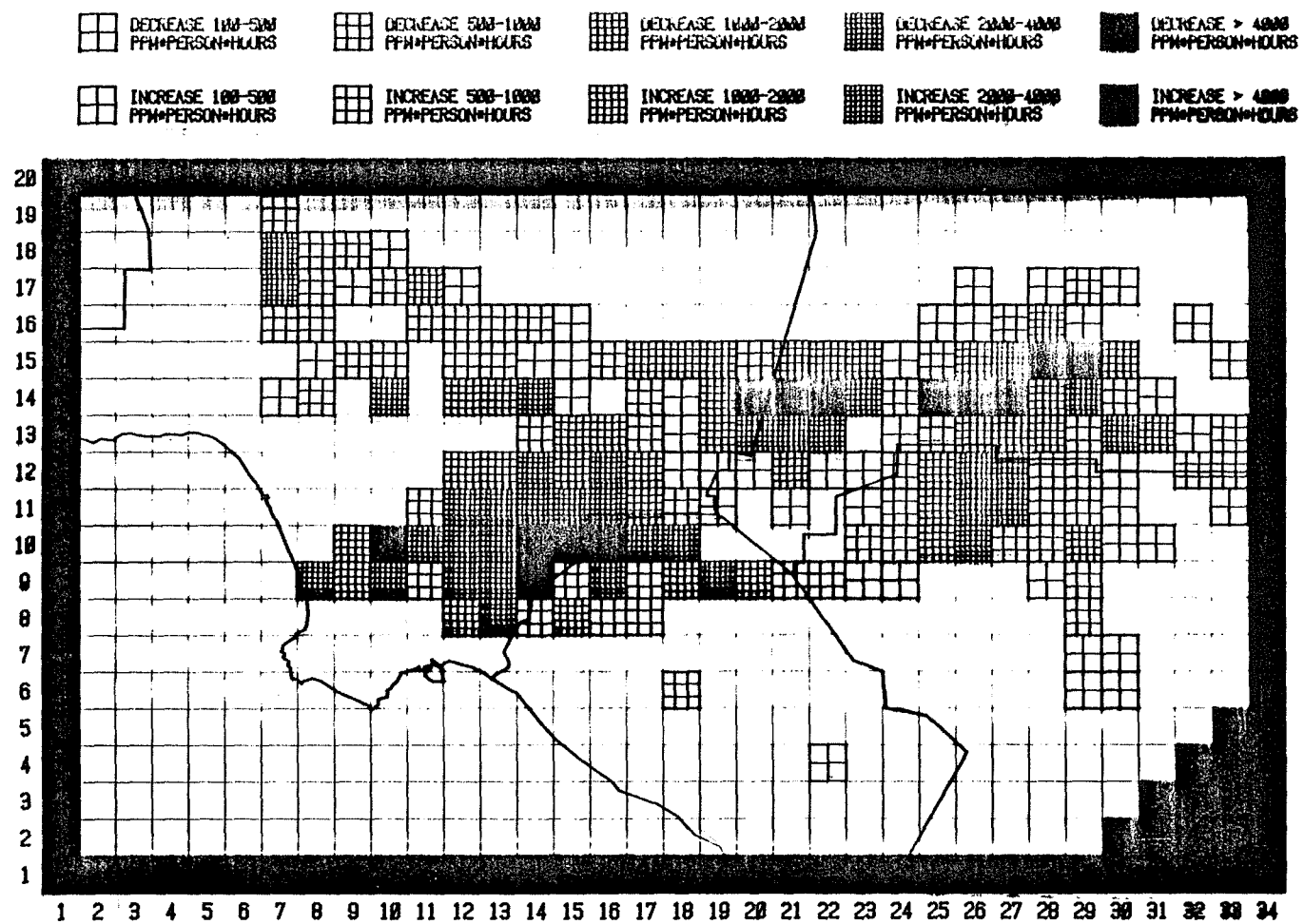


OZONE POTENTIAL EXPOSURE

$$\sum_{x=1}^{34} \sum_{y=1}^{20} \sum_{t=1}^{24} (C\ x, y, t, - Co)$$

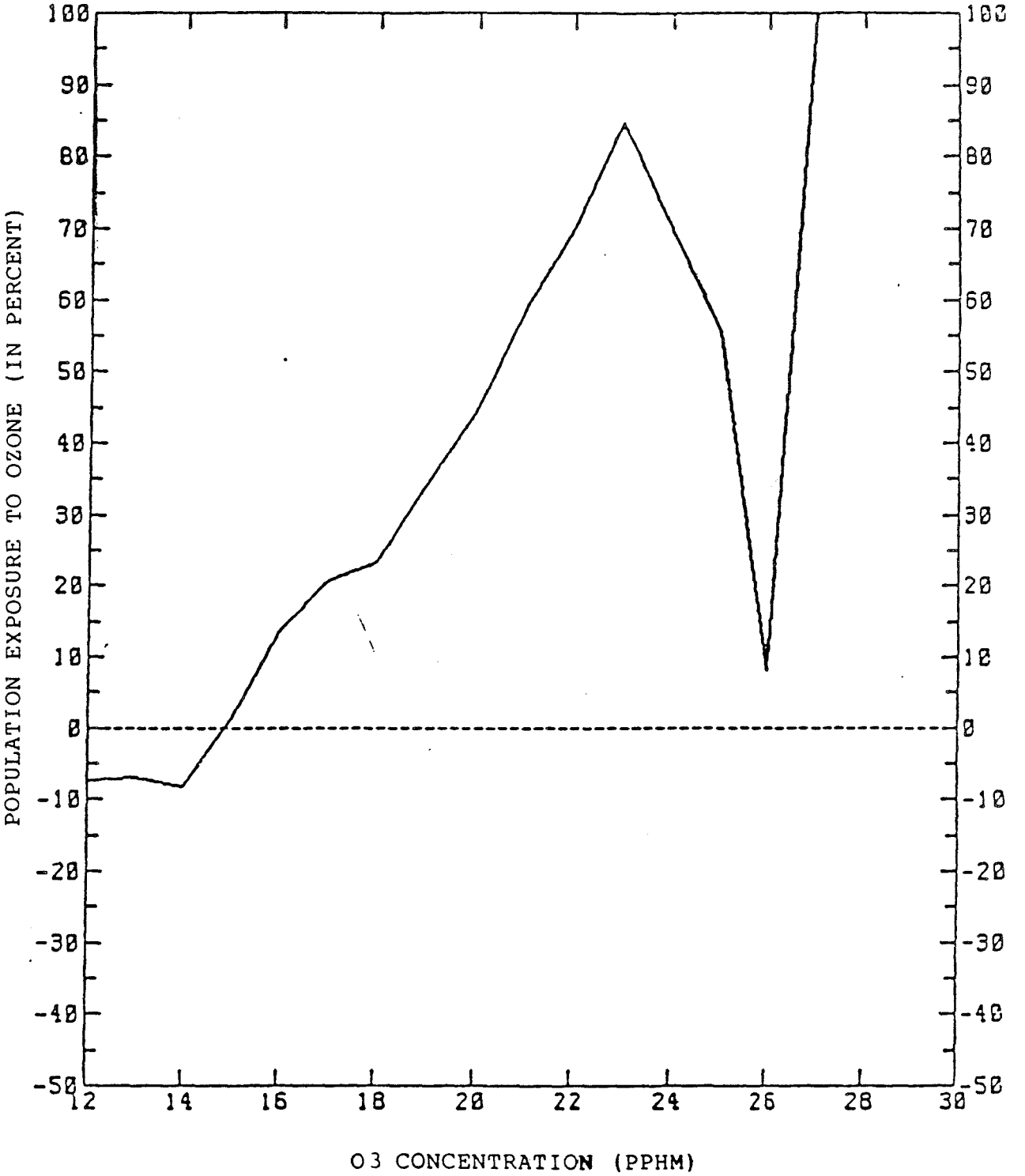
OZONE POPULATION EXPOSURE

$$\sum_{x=1}^{34} \sum_{y=1}^{20} \sum_{t=1}^{24} (C\ x, y, t, -Co) * Px, y$$

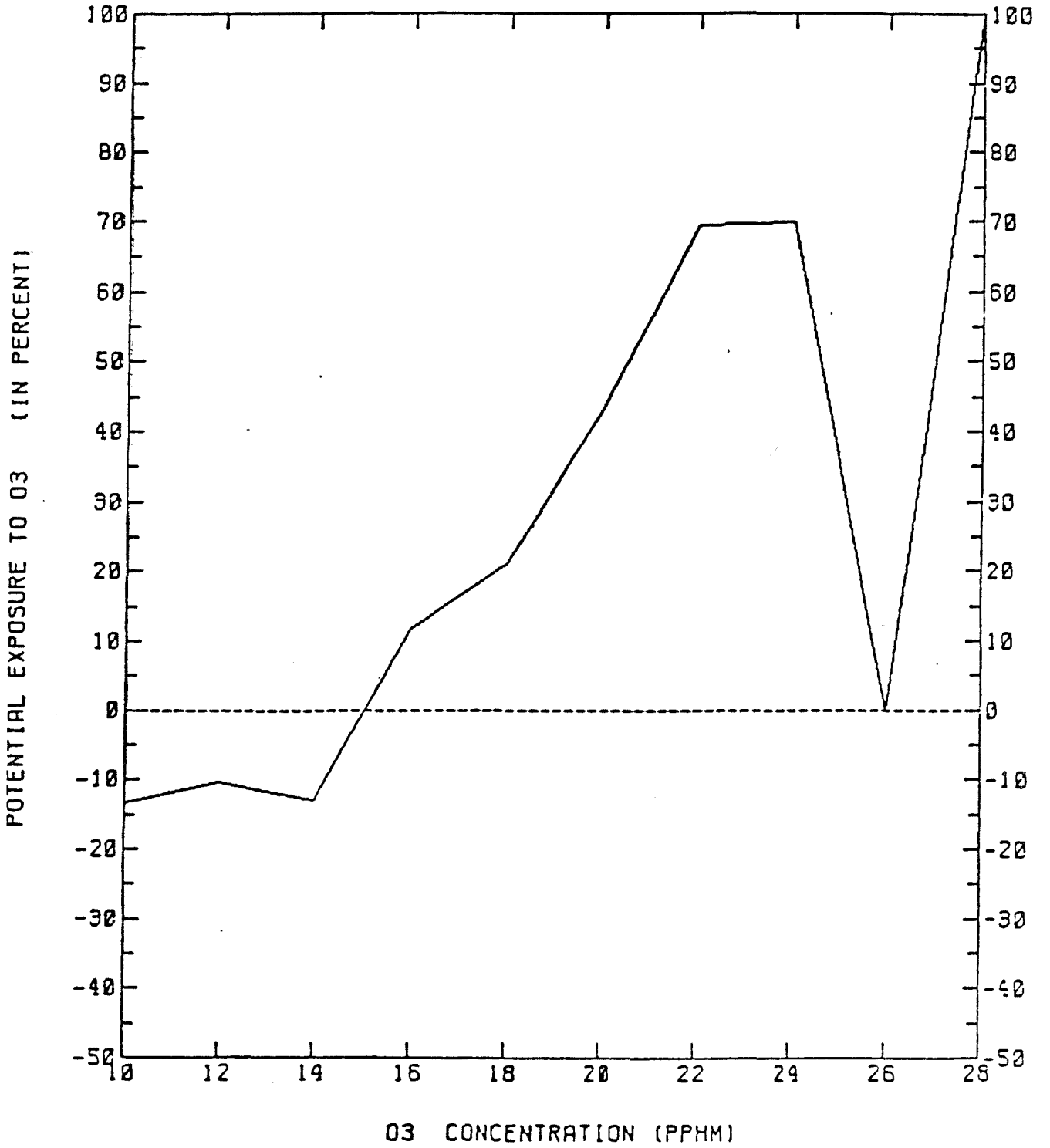


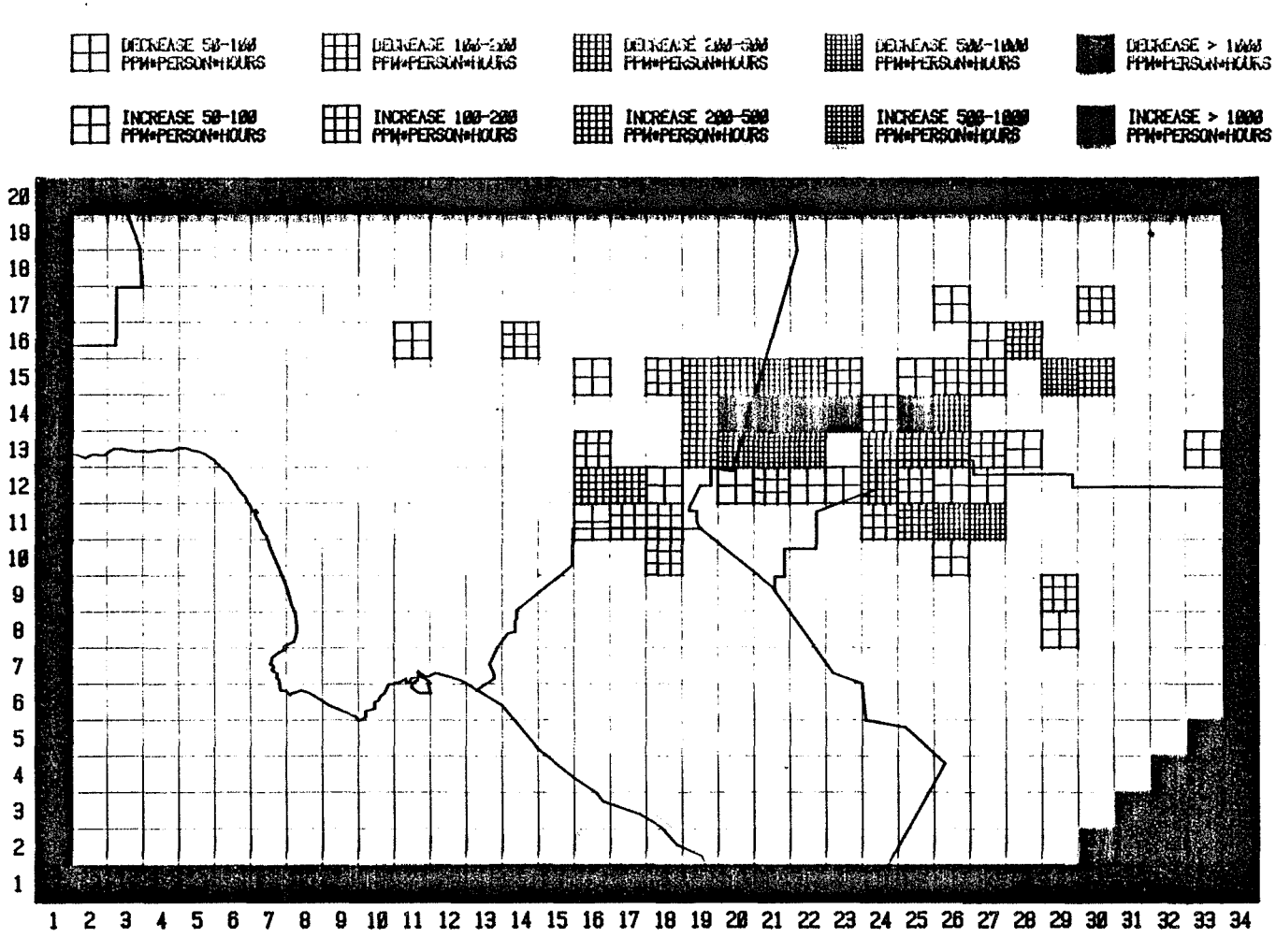
CHANGE IN OZONE EXPOSURE IN 1987 WITH THE IMPLEMENTATION OF SHORT-RANGE CONTROL MEASURES USING A THRESHOLD OF 0.12 PPM

CHANGES OF OZONE POPULATION EXPOSURE WITH THE IMPLEMENTATION OF AQMP CONTROL MEASURES



CHANGES OF OZONE POTENTIAL EXPOSURE WITH THE IMPLEMENTATION OF AQMP CONTROL MEASURES





CHANGE IN OZONE EXPOSURE IN 1987 WITH THE IMPLEMENTATION OF SHORT-RANGE CONTROL MEASURES USING A THRESHOLD OF 0.20 PPM

MAJOR CRITICISMS

(1) Prediction of Absolute Peak Concentration

(2) Representativeness of Single Episode

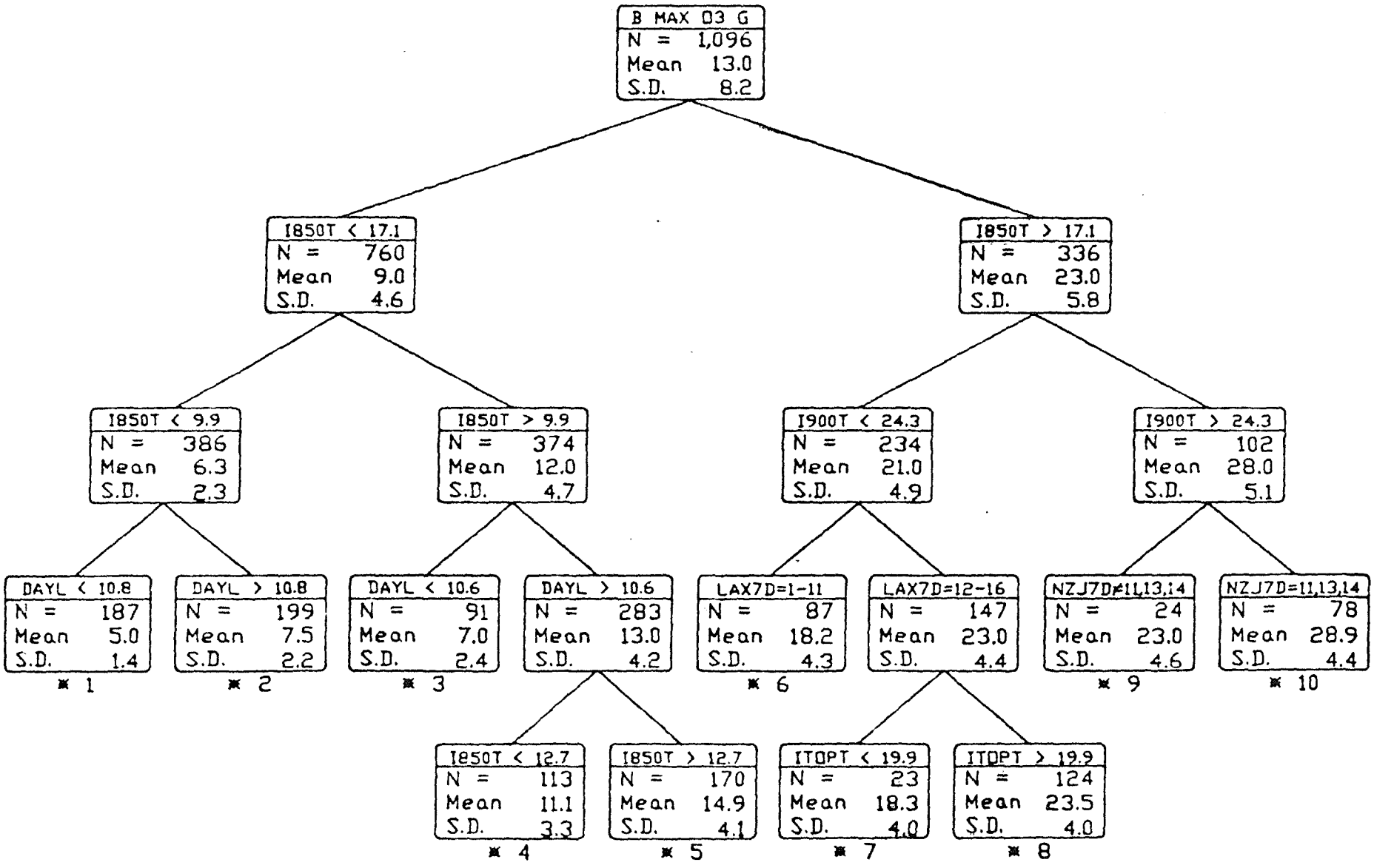
(3) Presentation of Basinwide Impacts

(4) Structure of Modeling Scenarios

METEOROLOGICAL VARIABLE USED IN CART ANALYSIS

Type	No.
Forecasting Pattern	**1**
Daylight Hours	1
Pressure Gradients	4
Inversion	7
Wind	56

RESULTS OF CART ANALYSIS



OZONE HEALTH INDEX

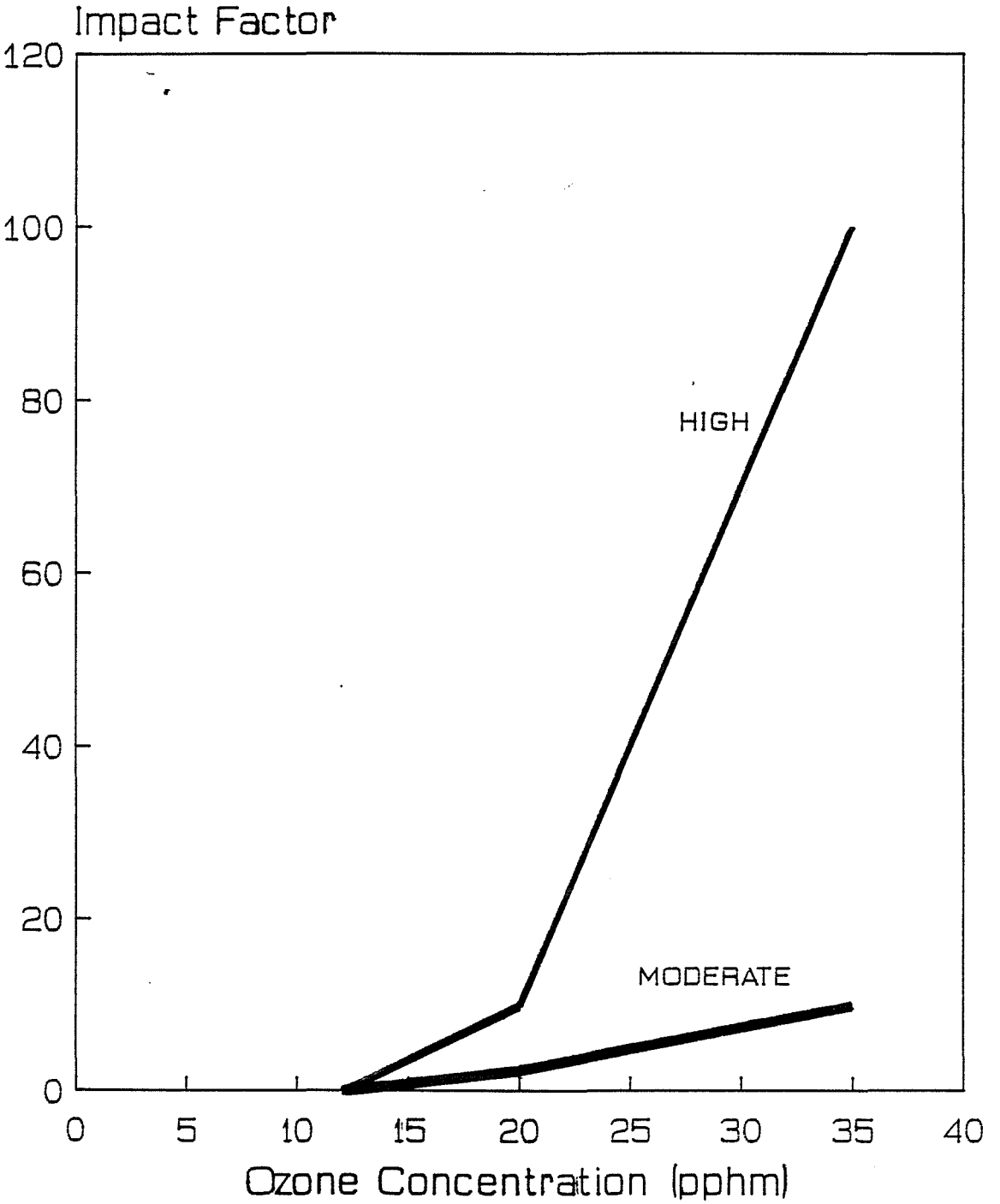
Exposure - Response Relationship

- 0 Lung Function (FEV1)
- 0 Lower Respiratory Symptom
  (Cough and Chest Discomfort)

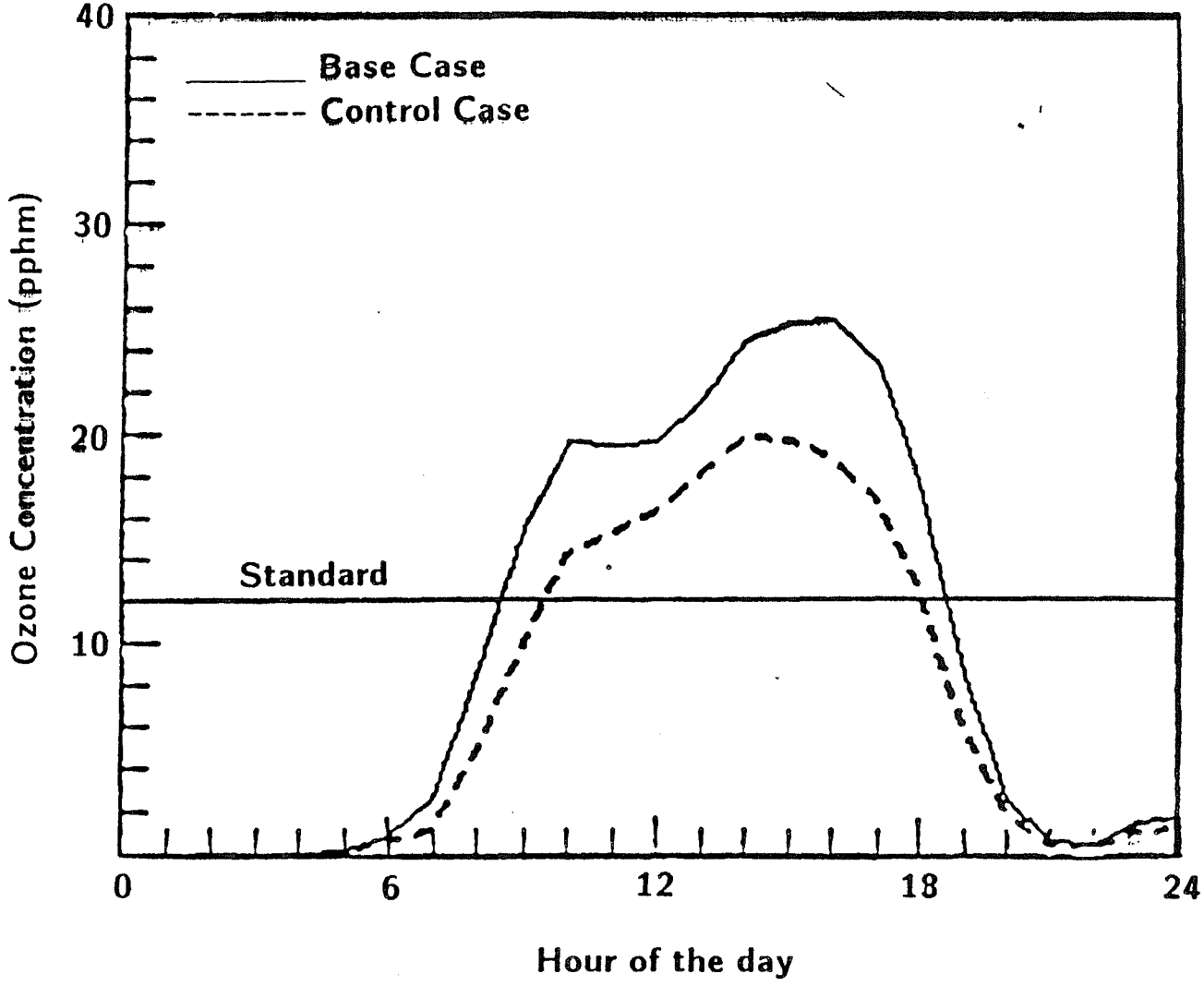
Health Risk

- 0 Benchmark Risk (Hazard)
- 0 Headcount Risk (Personal Exposure)

OZONE HEALTH IMPACT FACTOR



CHANGE OF DIURNAL PATTERN WITH CONTROL



COMPARISON OF EFFECTIVENESS OF CONTROL USING DIFFERENT AIR QUALITY MEASURES

Measure	Reduction (%)
Peak Ozone Concentration	23
Linear Dose-Response Model With Threshold	52
Health Index Model With Moderate Impact Factor	58
Health Index Model with High Impact Factor	76

OZONE AIR QUALITY INDEX

$$\left[\sum_{m=1}^{n} \left(\sum_{x=1}^{Xa} \sum_{y=1}^{Ya} \sum_{t=1}^{24} I(Cx, y, t,) \right) * Fm \right] / (Xa * Ya)$$

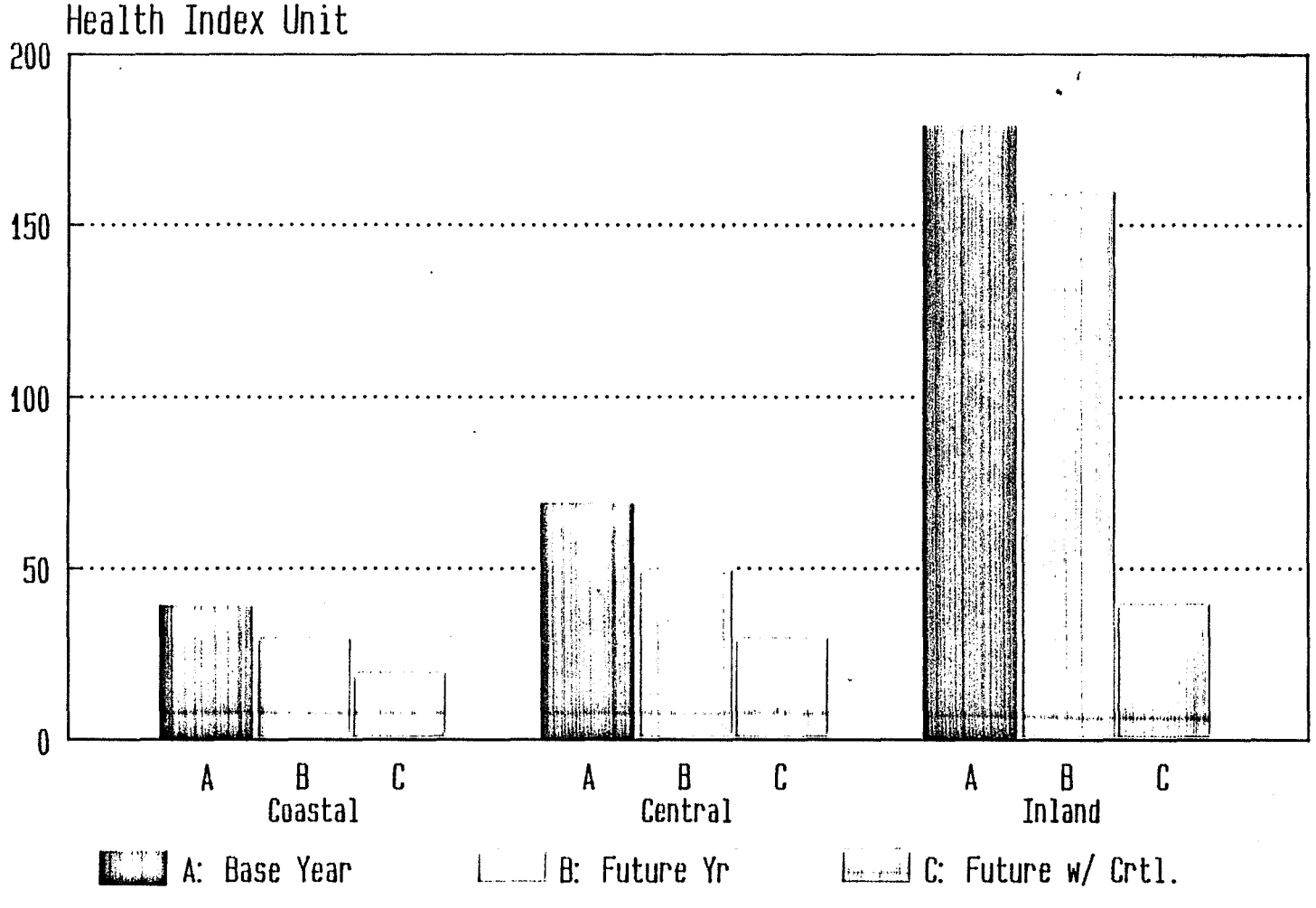
m: Meteorological Class

I: Impact Factor

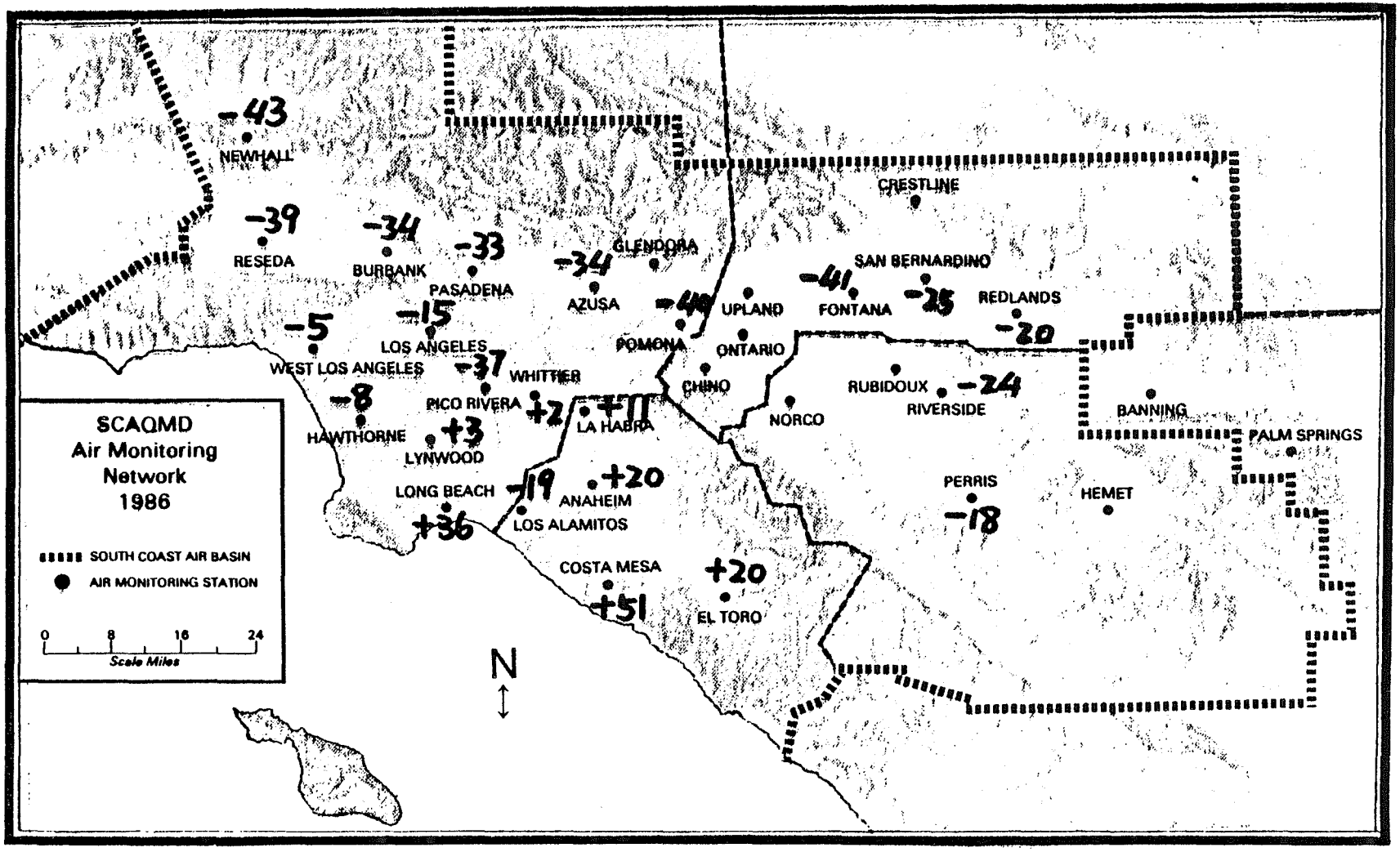
F: Frequency of Occurrence

Xa, Ya: Dimension of a Specific Area

HYPOTHETICAL RESULTS



CHANGES IN OZONE AIR QUALITY FROM 1976-1980 TO 1981-1985 IN THE SOUTH COAST AIR BASIN* (%)



* Assume linear dose-response and 12 pphm as threshold

ATTRIBUTES OF A BOUNDING CALCULATION

1. Overestimation of concentrations

2. Underestimation of changes in concentrations due to emissions reductions

3. Acceptable prior performance evaluation

4. Consistency in over- and underestimation

5. Target multiplier -- overprediction factor

6. Modification of model or inputs to assure over- or underprediction

ADDITIONAL OR MODIFIED ATTRIBUTES SUGGESTED FOR BOUNDING FOR PHOTOCHEMICAL MODELS FOR USE IN REGULATORY EVALUATION IN CALIFORNIA

1. Concentrate on bounding changes in concentration.

2. First establish high quality of performance over a range of conditions.

3. Keep the base can "as is".

4. Modify model inputs only.
   Modify for the control case only.

5. Control level is determined when smallest decrement in emissions meets requirement for changes in concentrations for all episodes studied.

6. Consider adopting more robust measures of adverseness of air quality in determining if air quality goals are likely to be attained.

CANDIDATE INPUT VARIABLES FOR ALTERATION

1. Boundary conditions - upwind and aloft

2. Emissions - VOC and NOx

3. Meteorological variables - mixing depth and winds

4. Chemical mechanisms

A PROPOSED APPROACH

1. Carry out performance evaluation - traditional requirements.

2. Select episodes of interest.

3. Determine input variables that are candidates for alteration.

4. Assess merits of altering each.

5. Determine patterns of alteration, including one-at-a-time, in pairs, etc.

6. Select conditions for bounding runs.

7. Subject choices to open review and scrutiny.

8. Alter plans, taking into account suggestions.

9. Carry out simulations.

ISSUES REQUIRING ATTENTION

1. Thoughtful development of procedure.

2. Rules for selecting episodes.

3. Selection of "bounding variables".

4. Procedures for estimating ranges of uncertainties in input variables.

5. Selection of measures for determining if objective is likely to be met.

6. Containing costs.

CONCLUDING OBSERVATIONS

1. Bounding appears to be feasible using photochemical models.

2. Development and testing of procedures now needed.

3. Judicious crafting to balance desire for conservatism and avoidance of unnecessary underestimation.

4. Bounding is not a short cut.

S. ZIMAN
Chevron USA

Data Aloft for Photochemical Modeling Applications

Photochemical Modeling as a Tool for Decision Makers

CARB/CIT

February 1988

I. Why is there a need to collect data aloft?

A. Physical—Ground measurements can't be extrapolated to data aloft.

B. Conceptual/Historical—Knowledge of aloft chemistry and meteorology is essential to understanding and modeling pollutant episodes.

C. Can lead to more effective control strategy development

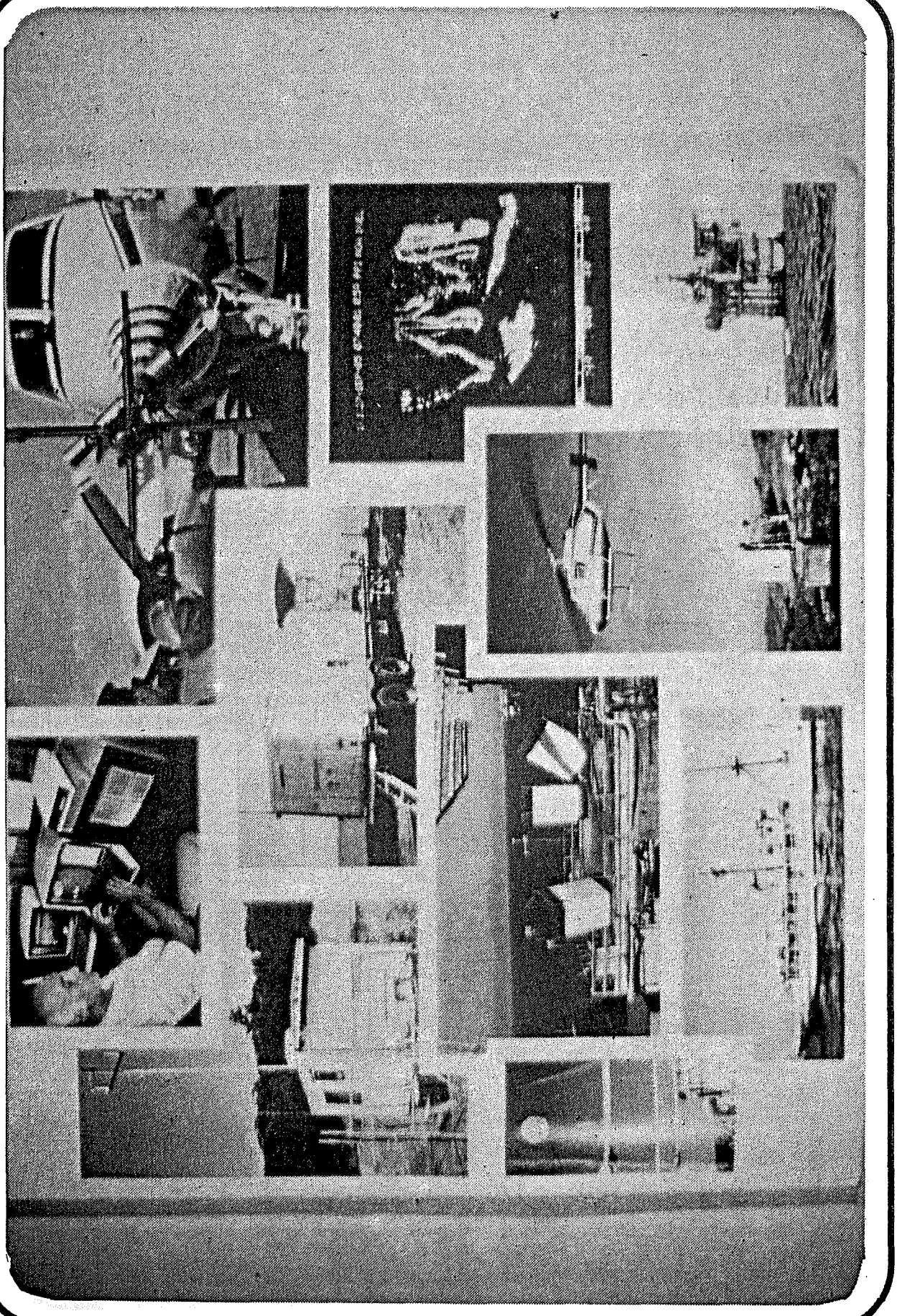
II. How are aloft model data needs met?

A. Stationary Platforms

- Doppler acoustic sounders
- Doppler radar
- Tall towers
- Collection at high terrain sites
- Stationary balloons

B. Mobile Platforms

- Airplanes and helicopters
- Pibal, radiosondes, tetroons
- Boats
- Tracers



III. Are current systems adequate?

A. Instantaneous/semi-instantaneous measurements are used to develop hourly averages for model input. Is this acceptable?

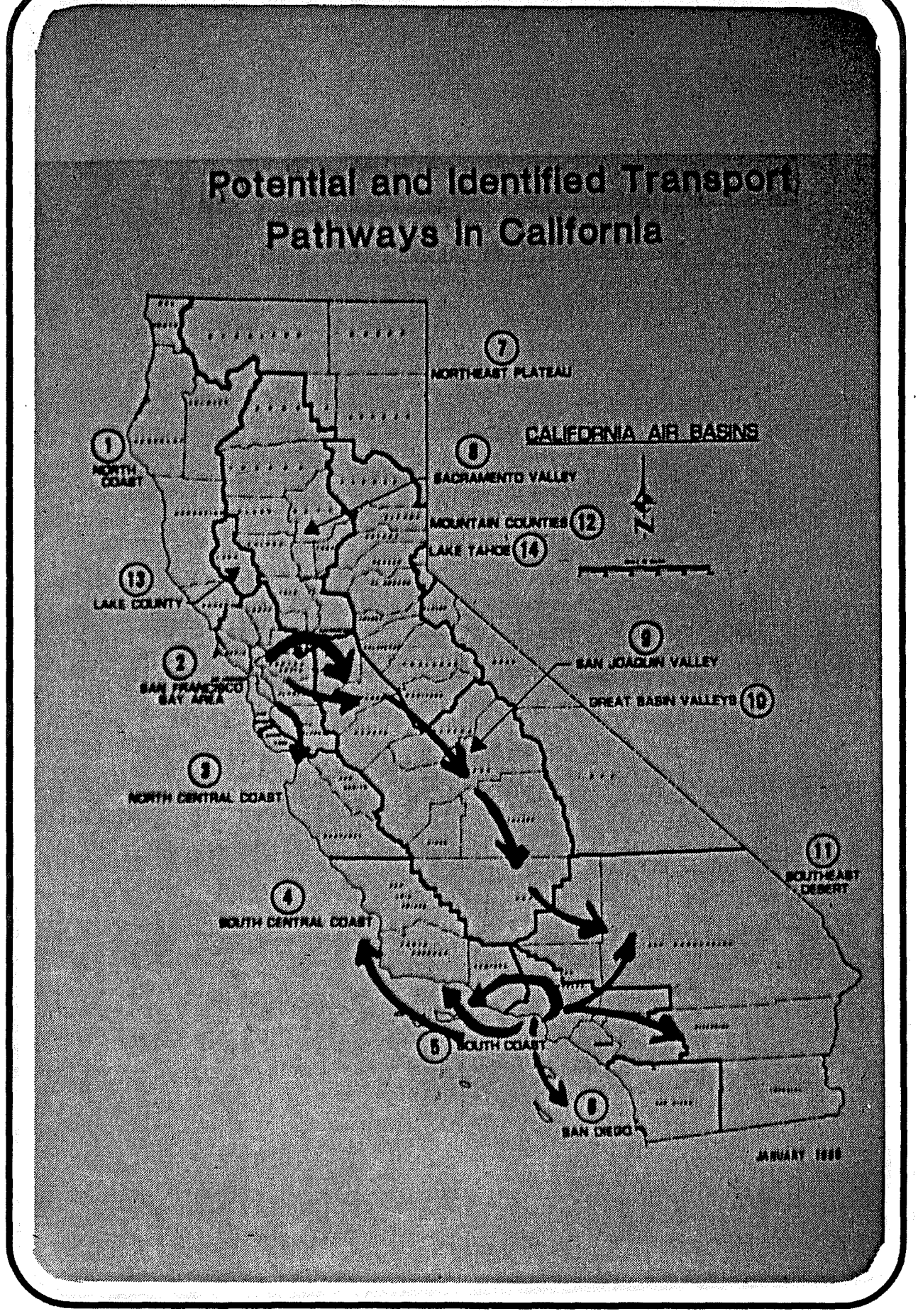
B. Are measurements representative of geographical area for model input and performance evaluation?

C. What are tradeoffs between number of measurements and cost?

IV. Can measurements be improved?

A. Two issues
   1. Improve the timing, location, and number of measurements.
   2. Improve methodologies.

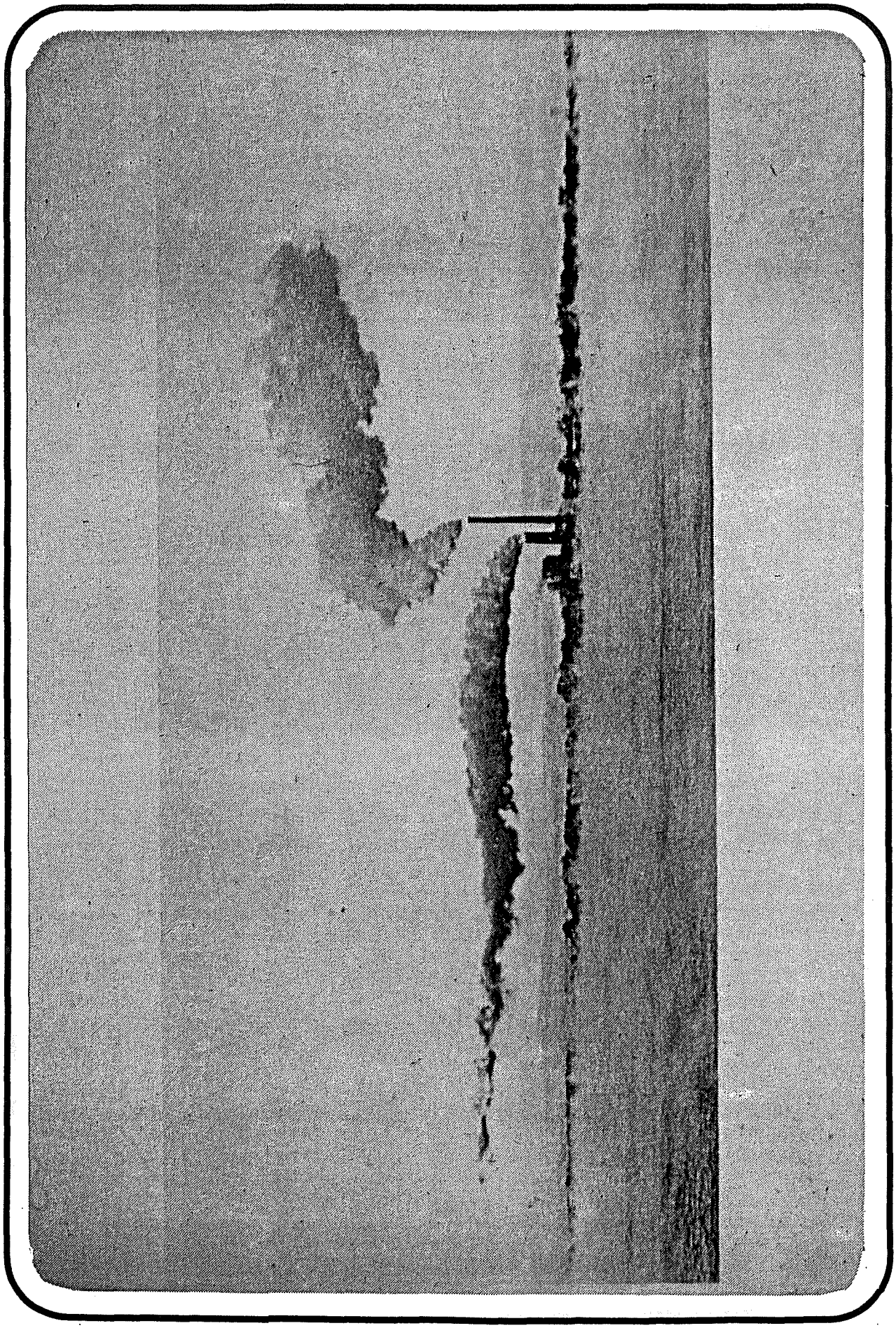
B. Are improved measurements cost-effective relative to improvements in model performance?


Potential and Identified Transport Pathways In California
CALIFORNIA AIR BASINS
7 NORTHEAST PLATEAU
1 NORTH COAST
8 SACRAMENTO VALLEY
MOUNTAIN COUNTIES 12
LAKE TAHOE 14
13 LAKE COUNTY
9 SAN JOAQUIN VALLEY
2 SAN FRANCISCO BAY AREA
GREAT BASIN VALLEYS 10
3 NORTH CENTRAL COAST
11 SOUTHEAST DESERT
4 SOUTH CENTRAL COAST
5 SOUTH COAST
6 SAN DIEGO
JANUARY 1988

V. How can aloft data influence control strategy decisions?

1. Distinguish between local and transported precursors and transported ozone, and determine their effects on control strategy selection.

2. Compare effectiveness of NOx controls for ground-level and elevated emission sources.



Summary

Aloft data needed to:

- Improve model performance
- Lead to better understanding of ozone formation
- Provide basis to design more effective control strategies

Session IV
Interpretation Of Results

2 February 1988

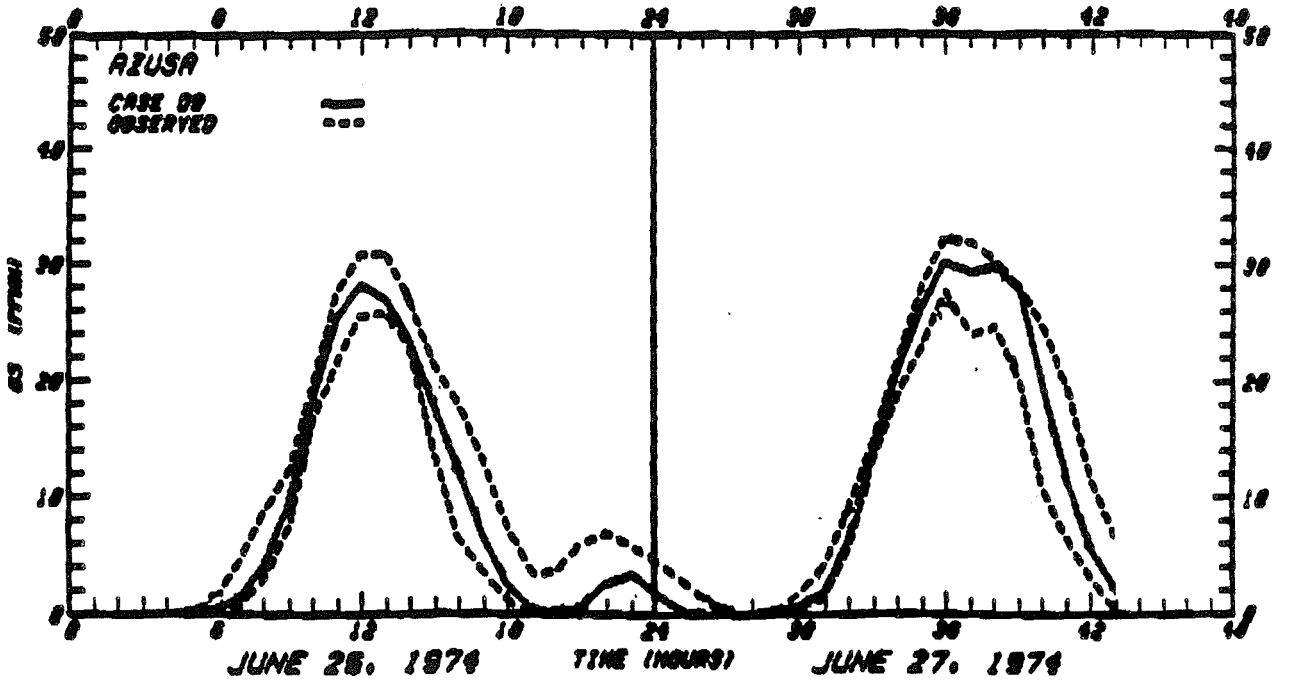
8:30 – 10:00

Model Performance Concepts

- **Model Calibration** – Adjustment of Empirical Model Constants or Parameters to Optimize Agreement Between Prediction and Observation.
- **Model Validity** – Degree of Agreement Between Model Predictions and Observations, Given Perfect Model Inputs.
- **Model Evaluation** – Process of Examining and Quantifying Performance.
- **Model Varification** – Successful Evaluation of the Model.

Model Performance Issues

- Accuracy of Peak Prediction (Various Definitions).
- Bias and Imprecision.
- Model Performance Where Emissions Have Greatest Impact.
- Adequacy of NO, NO_2, RHC Predictions.
- Time and Space Correlation.
- Modeled, Measured, and Inventory RHC/NO_X Ratios.
- Representitiveness and Uncertainty.



Hypothetical Comparison Between Ozone Predictions And Measurement Uncertainty Bounds.

Summary of Ozone Predictions

Single Day Simulations

- Average error is 35%
- Average bias is −10%
- 44 of 63 cases (70%) reveal underprediction
- California studies slightly more accurate (35% vs. 41%)
- Coastal simulations slightly more accurate (31% vs. 38%)

Summary (Continued)

Multiple-Day Simulations

- Average error is 37%
- Average bias is +5%
- 6 of 10 cases (60%) reveal underprediction
- No apparent change in accuracy between coastal vs. inland cities

Summary (Concluded)

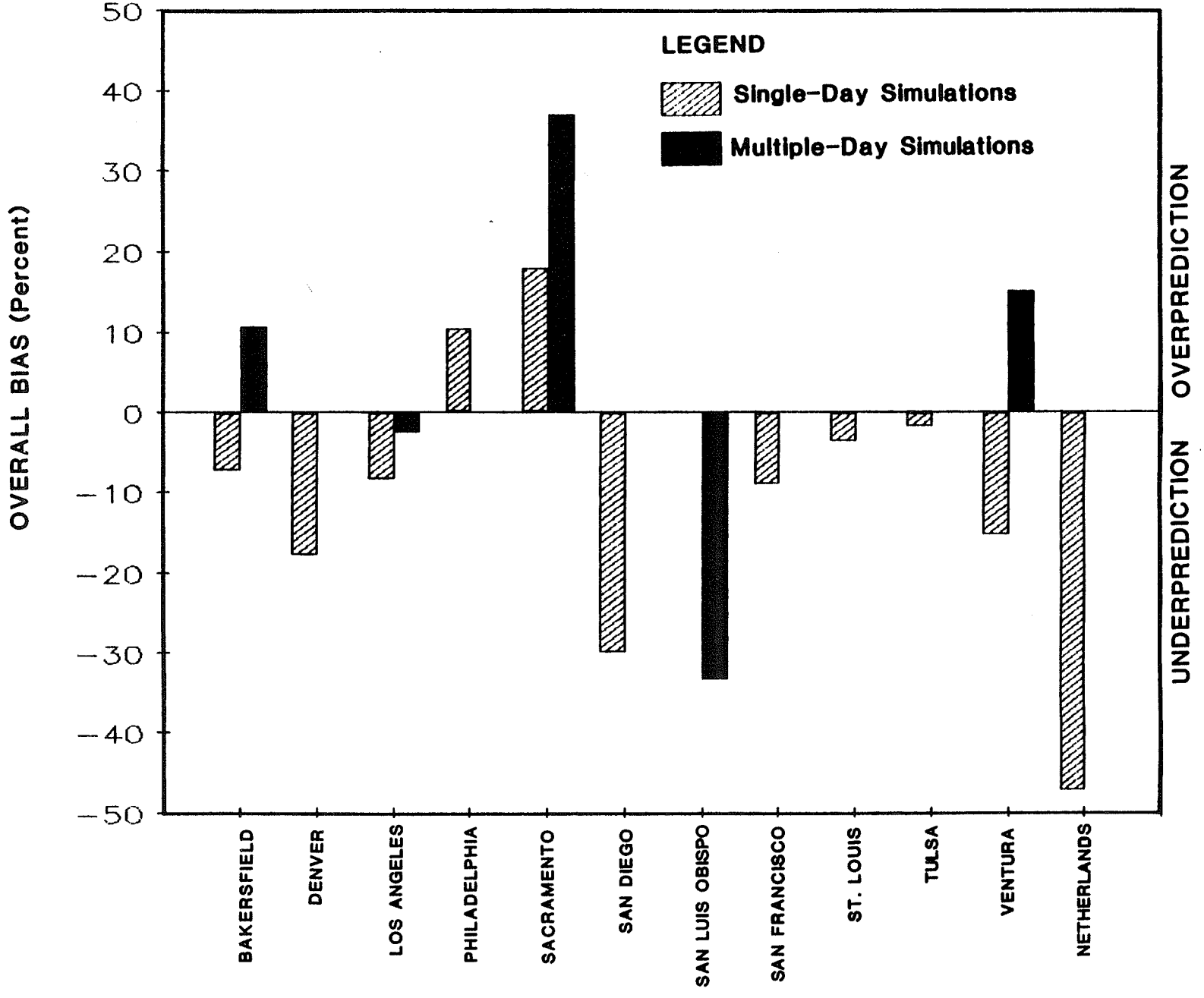
Temporal/Spatial Pairing

- Relaxing requirement for time/space pairing in St. Louis simulations reduced bias from −32% to +4%

Conclusions

- The overall accuracy of photochemical grid models is 35-40% (paired in time and space).
- Errors in single day simulations are somewhat less than for multiple day runs.
- Grid models ozone predictions tend to be biased low.

FIGURE 1. OVERALL BIAS IN HOURLY-AVERAGED OZONE PREDICTIONS BY URBAN AREA



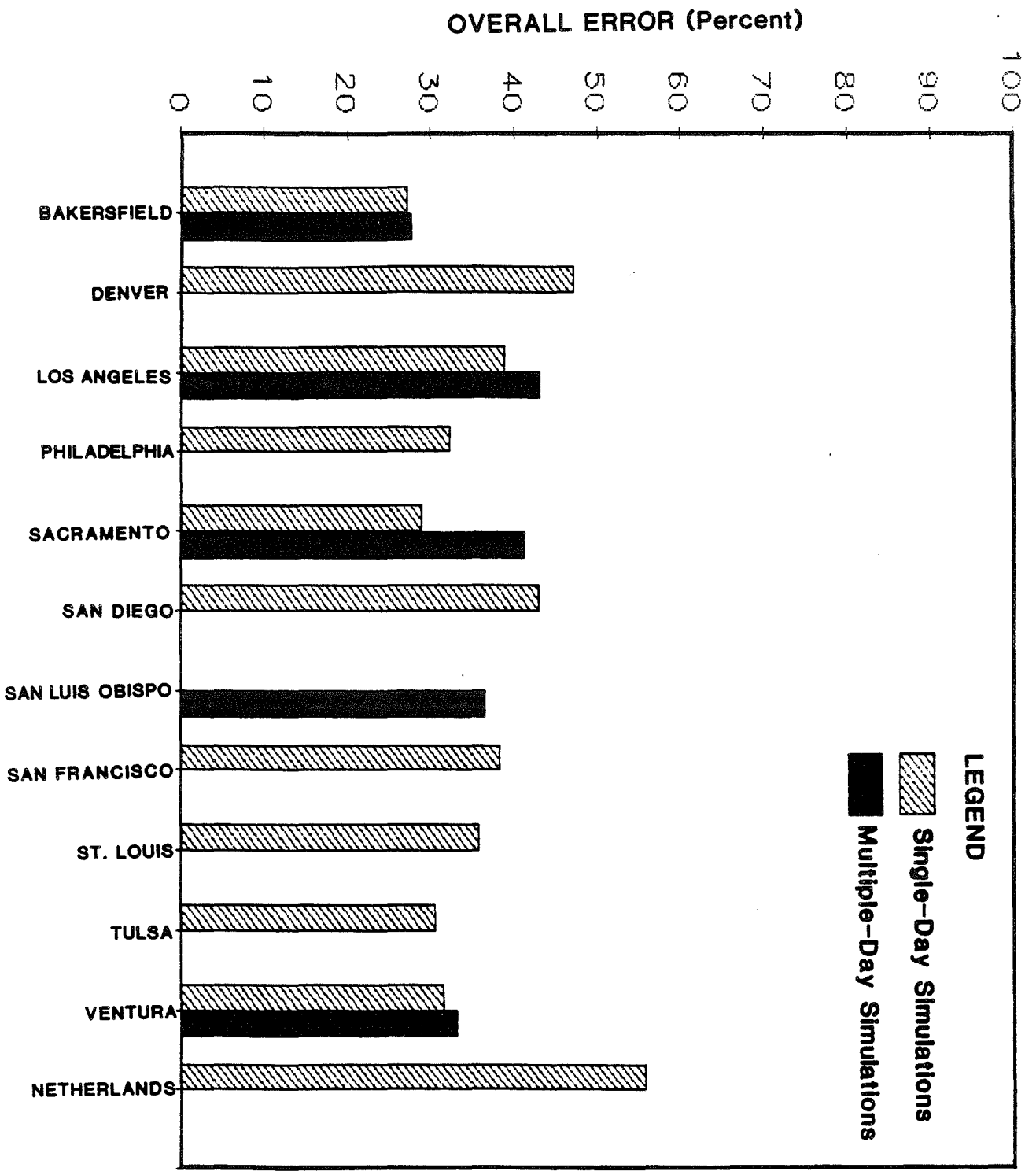


FIGURE 2. OVERALL GROSS ERRORS IN HOURLY-AVERAGED OZONE PREDICTIONS BY URBAN AREA

Table 3. Grid Model Bias in Hourly Average Ozone Predictions

Urban Area	Single Day		Multiple-Day	
	Bias (percent)	No. of Simulations	Bias (percent)	No. of Simulations
Bakersfield	−7.3	6	10.7	1
Denver	−17.8	13	—	—
Los Angeles	−8.4	6	−2.6	3
Philadelphia	10.5	2	—	—
Sacramento	18.0	3	37.0	1
San Diego	−30.0	1	—	—
San Francisco	−9.0	1	—	—
San Luis Obispo	—	—	−33.5	2
St. Louis	−3.7	20	—	—
Tulsa	−1.8	4	—	—
Ventura-Santa Barbara	−15.3	6	15.2	3
The Netherlands	−47.3	1	—	—

Table 4. Grid Model Error in Hourly Average Ozone Predictions

Urban Area	Single Day		Multiple-Day	
	Error (percent)	No. of Simulations	Bias (percent)	No. of Simulations
Bakersfield	27.4	6	27.9	1
Denver	47.3	13	—	—
Los Angeles	39.1	6	43.3	3
Philadelphia	32.5	2	—	—
Sacramento	29.2	3	41.4	1
San Diego	43.1	1	—	—
San Francisco	38.4	1	—	—
San Luis Obispo	—	—	36.7	2
St. Louis	36.0	20	—	—
Tulsa	30.8	4	—	—
Ventura-Santa Barbara	31.7	6	33.3	3
The Netherlands	55.9	1	—	—

POTENTIAL SOURCES OF OZONE UNDERESTIMATION

- Horizontal grid resolution
- Vertical grid resolution
- Volume averaging
- Subgrid scale phenomena
- Treatment of carryover
- Numerical error
- Deposition velocities
- Emission inventory
- Hydrocarbon AQ data
- Nighttime chemistry

Performance Evaluation: Needs And Future Directions

by

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presented at

Photochemical Modeling as a Tool for Decision Makers
1-3 February 1988
California Institute of Technology
Pasadena, CA

Outline Of Presentation

- Current Model Evaluation Procedures
- Specific Areas Where Refinement is Needed
- Recommendations

Photochemical Grid Models Used in Urban Ozone Applications

- Airshed
- CALTECH
- LIRAQ
- PARIS
- SMOG

Urban Areas Examined with Photochemical Grid Models

- Bakersfield, California
- Denver, Colorado
- Los Angeles, California
- Philadelphia, Pennsylvania
- Sacramento, California
- San Diego, California
- San Luis Obispo, California
- St. Louis, Missouri
- Tulsa, Oklahoma
- Ventura-Santa Barbara, California
- Netherlands, Belgium and Germany

Model Evaluation Measures

- Accuracy of the Peak Ozone Prediction
- Bias
- Absolute Error
- Temporal, Spatial Correlation

Four Types Of Pairing For Accuracy Estimation

- Paired in Time and Space
- Paired in Time but Not Space
- Paired in Space but Not Time
- Unpaired in Time and Space

Statistical Performance Measures

- Concentration Residual $$d = C_o(x_1\ T) - C_p(x_1\ T)$$

- Bias $$\bar{d} = \frac{1}{N}[\Sigma(C_o(x_1\ T) - C_p(x_1\ T)]$$

- Gross Error $$|\bar{d}| = \frac{1}{N_N}\Sigma|d|$$

- Variance $$S_d^2 = \frac{1}{N-1}\ \Sigma(d-d)^{-2}$$

Graphical Performance Measures

- Scatter Plots of Observations Versus Predictions
- Time Series Plots of Predictions Versus Observations
- Ground-Level Concentrations Isopleths
- Bias Plots as a Function of Concentration Level
- Error Plots as a Function of Concentration Level
- Cumulative Frequency Distribution Plots of Observed and Predicted Concentrations
- Distribution of Distances to Bracket Observation

- Accuracy of Maximum 1-Hour Average Ozone Concentration (Unpaired in Time and Space)

Accuracy of the Peak PARIS Model Ozone Prediction

	11 Sept.	12 Sept.	25 Sept.	26 Sept.	28 Sept.	29 Sept.
Peak prediction	15.7 pphm	10.2 pphm	13.8 pphm	10.8 pphm	13.9 pphm	10.8 pphm
Peak station measurement	12.0 pphm (Piru)	18.0 pphm (Piru)	18.0 pphm (S. Mtn.)	16.0 pphm (Piru)	12.0 pphm (Piru)	18.0 pphm (Piru)
Error	31%	−43%	−23%	−33%	16%	−40%

- Accuracy of Ozone Predictions at Specific Monitors (Paired in Space)

Accuracy of PARIS Model Ozone Predictions at Specific Monitors

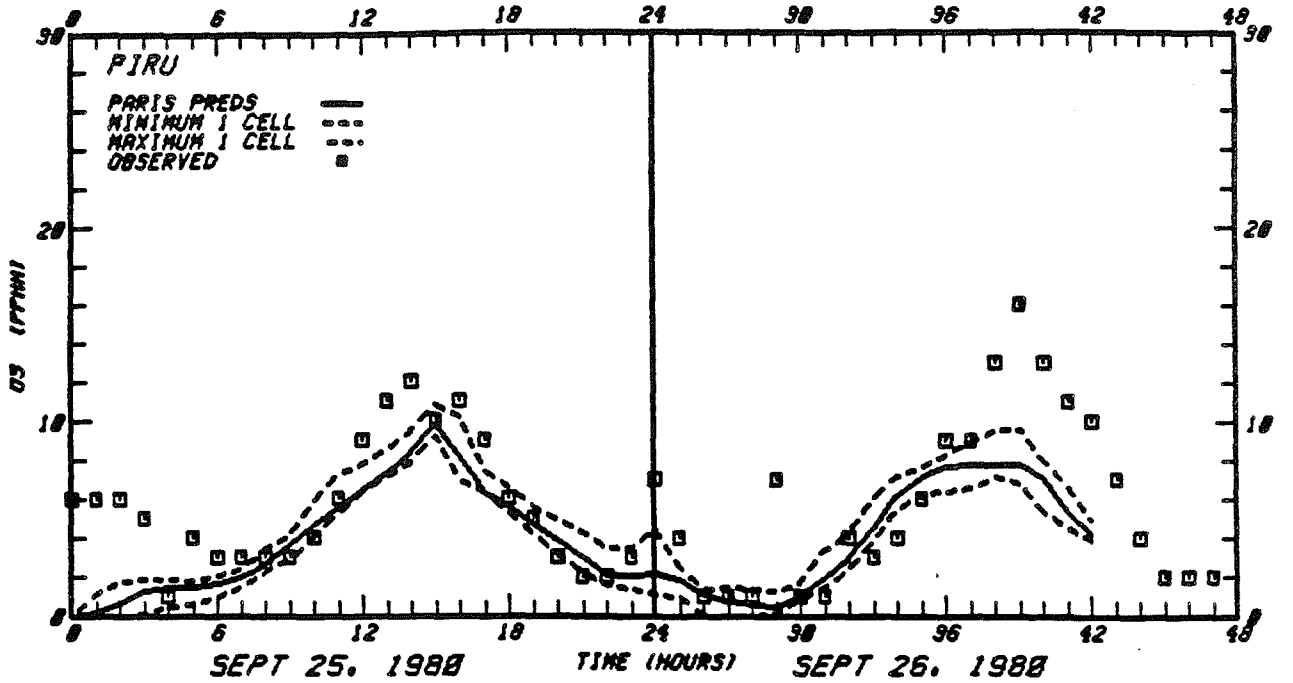
Stations	11 Sept. Percentage Difference	12 Sept. Percentage Difference	25 Sept. Percentage Difference	26 Sept. Percentage Difference	28 Sept. Percentage Difference	29 Sept. Percentage Difference
El Rio	2	−33	–	–	−5	−20
Grace	15	−30	–	–	−7	−6
Casitas	–	–	−24	−13	–	–
Moorpark	42	−33	52	−26	−12	–
Ojai	−28	−49	−37	−58	−88	−38
Piru	−1	−48	−15	−50	−22	−44
Simi	33	−34	18	−37	–	−40
S. Mountain	–	–	−31	−48	–	–

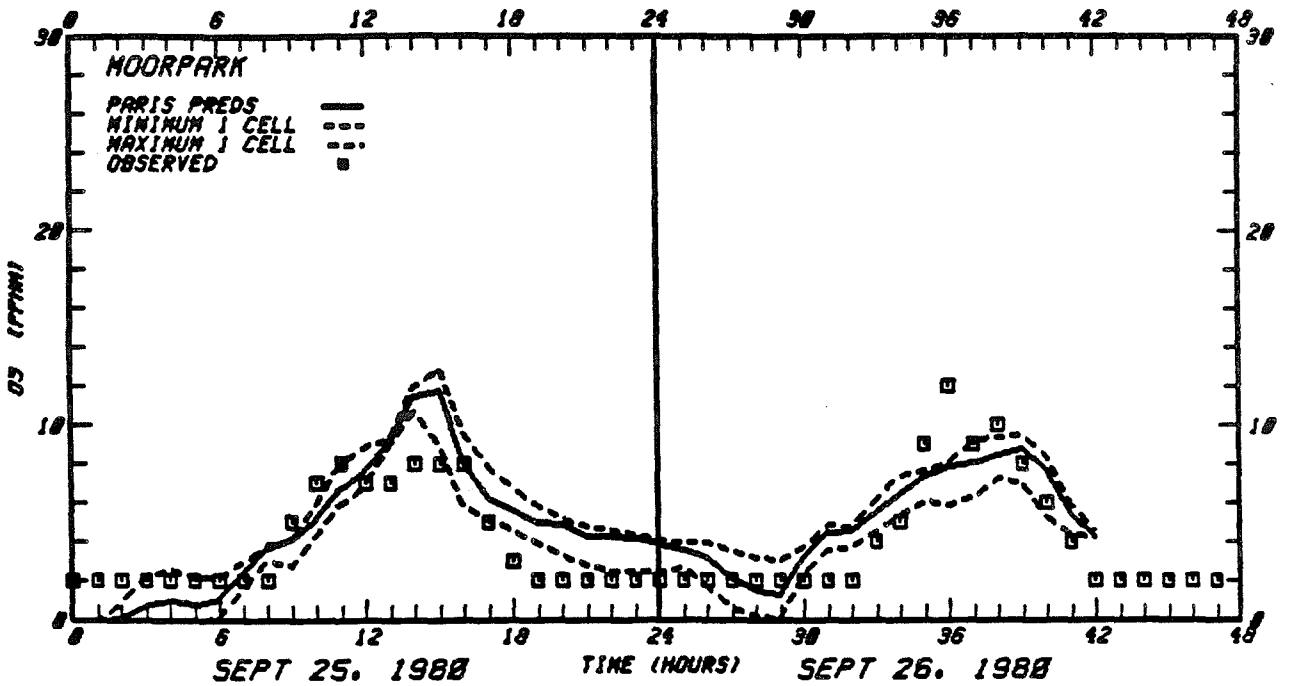
- Overall Bias and Absolute Error (Paired in Time and Space)

Overall Bias and Absolute Error Estimates for PARIS Model (Percent)

	11 Sept.	12 Sept.	25 Sept.	26 Sept.	28 Sept.	29 Sept.
Bias	−10.6	−32.2	−10.6	−8.1	−14.9	−15.2
Absolute Error	38.3	27.8	35.1	34.8	26.1	27.8

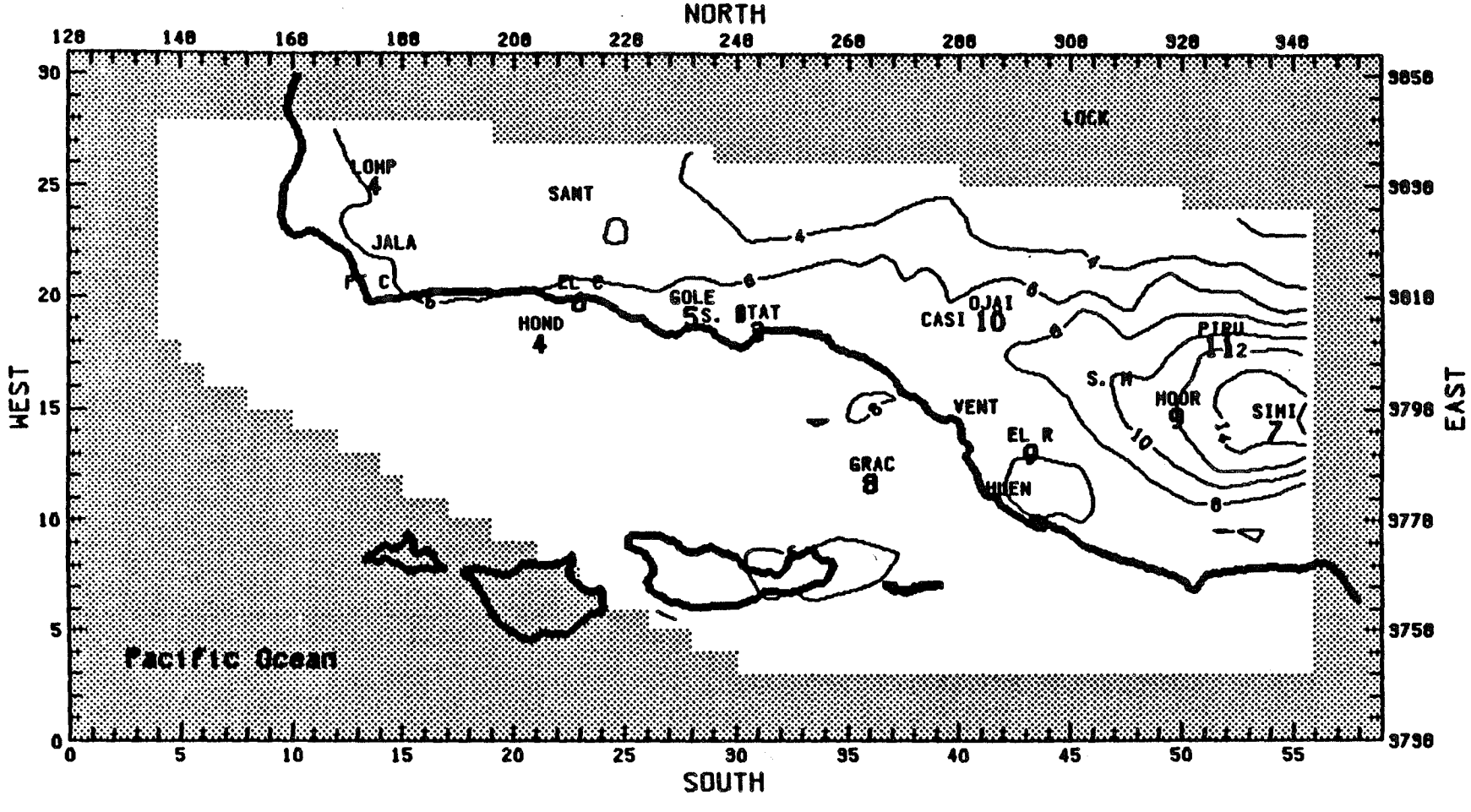
- Temporal Correlation



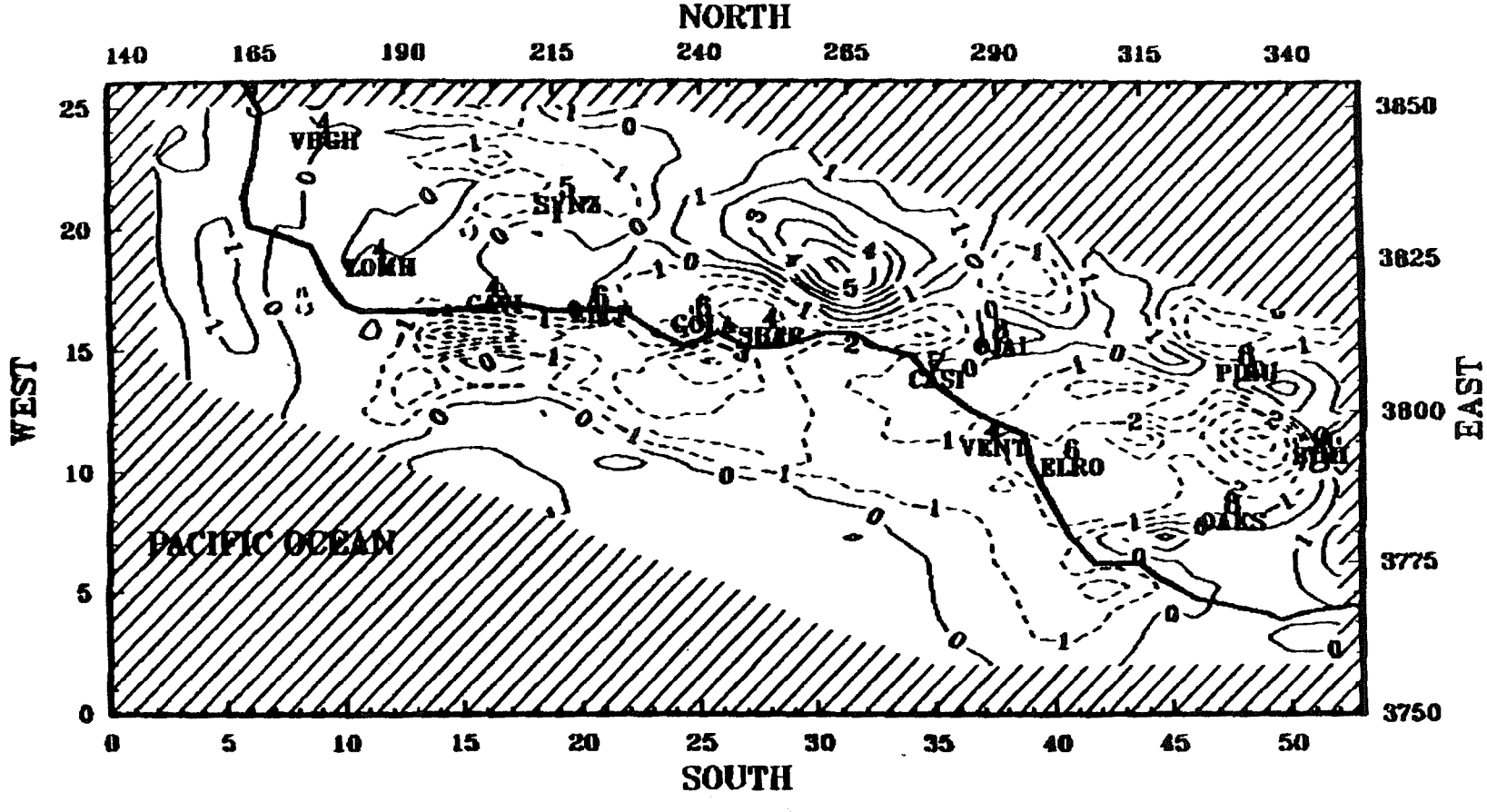


Time Series Plots of Predicted and Observed Ozone Concentrations for 25-26 September 1980.

- Spatial Correlation



Predicted Ground Level Ozone Concentration Fields for 11 September 1980, Between the Hours of 1400 and 1500.



Ozone Deficit-Enhancement Plot for 16 September 1984 in the South Central Coast Air Basin.
(Caltech Wind Fields Minus Diagnostic Windfields; pphm)

INTERPRETATION OF PHOTOCHEMICAL MODELING RESULTS

BY

KIT K. WAGNER

AIR QUALITY MODELING SECTION
TECHNICAL SUPPORT DIVISION
CALIFORNIA AIR RESOURCES BOARD

PRESENTED AT

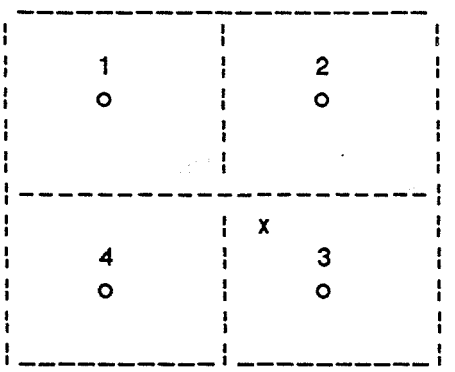
PHOTOCHEMICAL MODELING AS A TOOL FOR DECISION MAKERS

February 1-3, 1988 at the California Institute of Technology

GRAPHICAL PRESENTATIONS OF THE RESULTS OF PHOTOCHEMICAL MODELING CAN BE USED TO EVALUATE MODEL PERFORMANCE AND THE UNCERTAINTY OF MODELING RESULTS.

TYPES OF GRAPHS:

* STATION PLOTS
* ISOPLETH PLOTS
* SCATTER PLOTS
* RESIDUAL PLOTS
* DIFFERENCE PLOTS

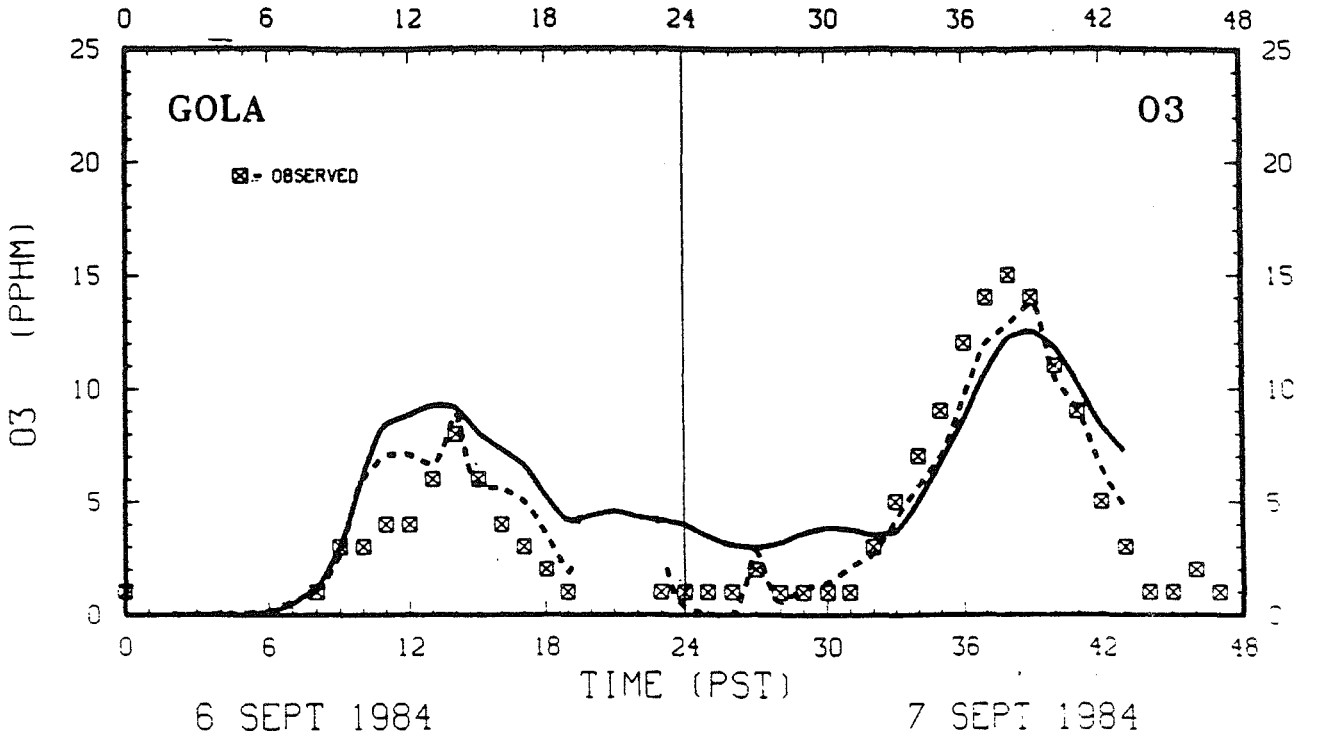


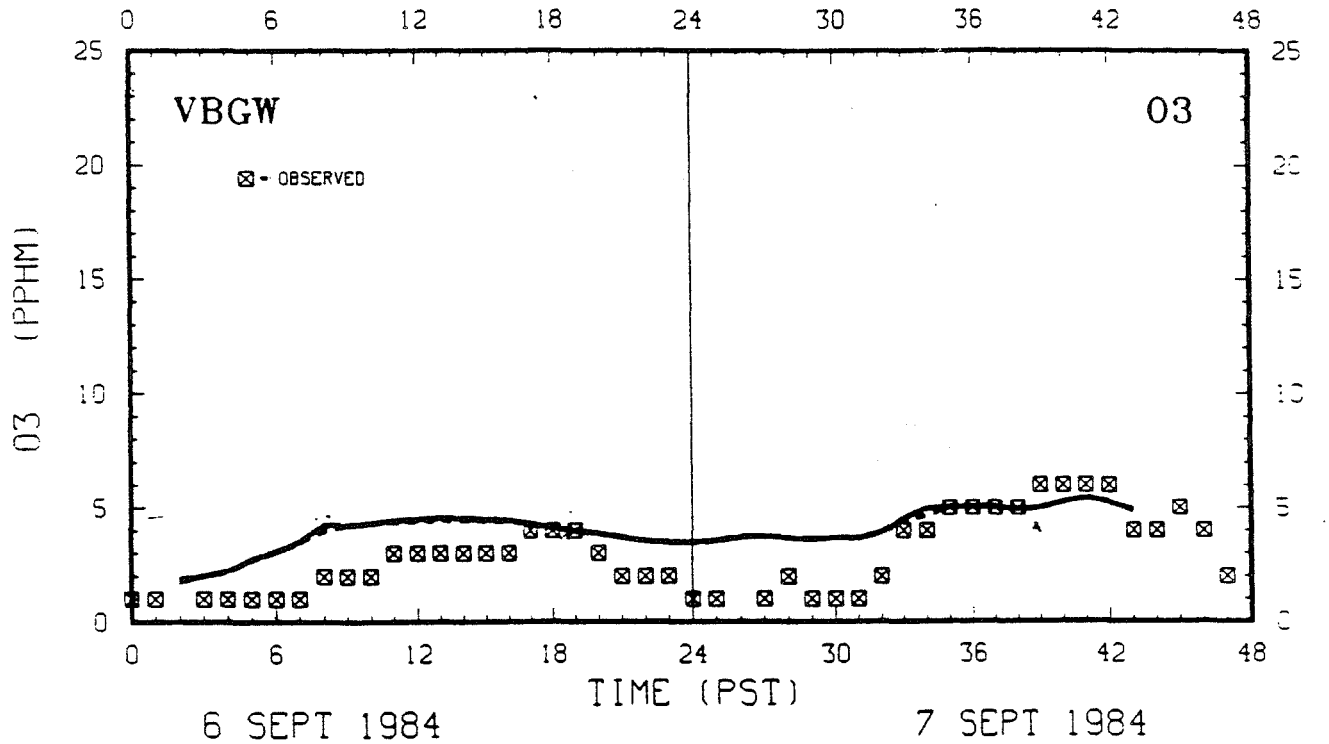
GRID CELL PREDICTIONS AT o ARE COMPARED TO OBSERVATIONS AT x

1. COMPARE THE OBSERVATION AT x TO THE CELL VALUE o_3 WHICH IS CLOSEST TO x

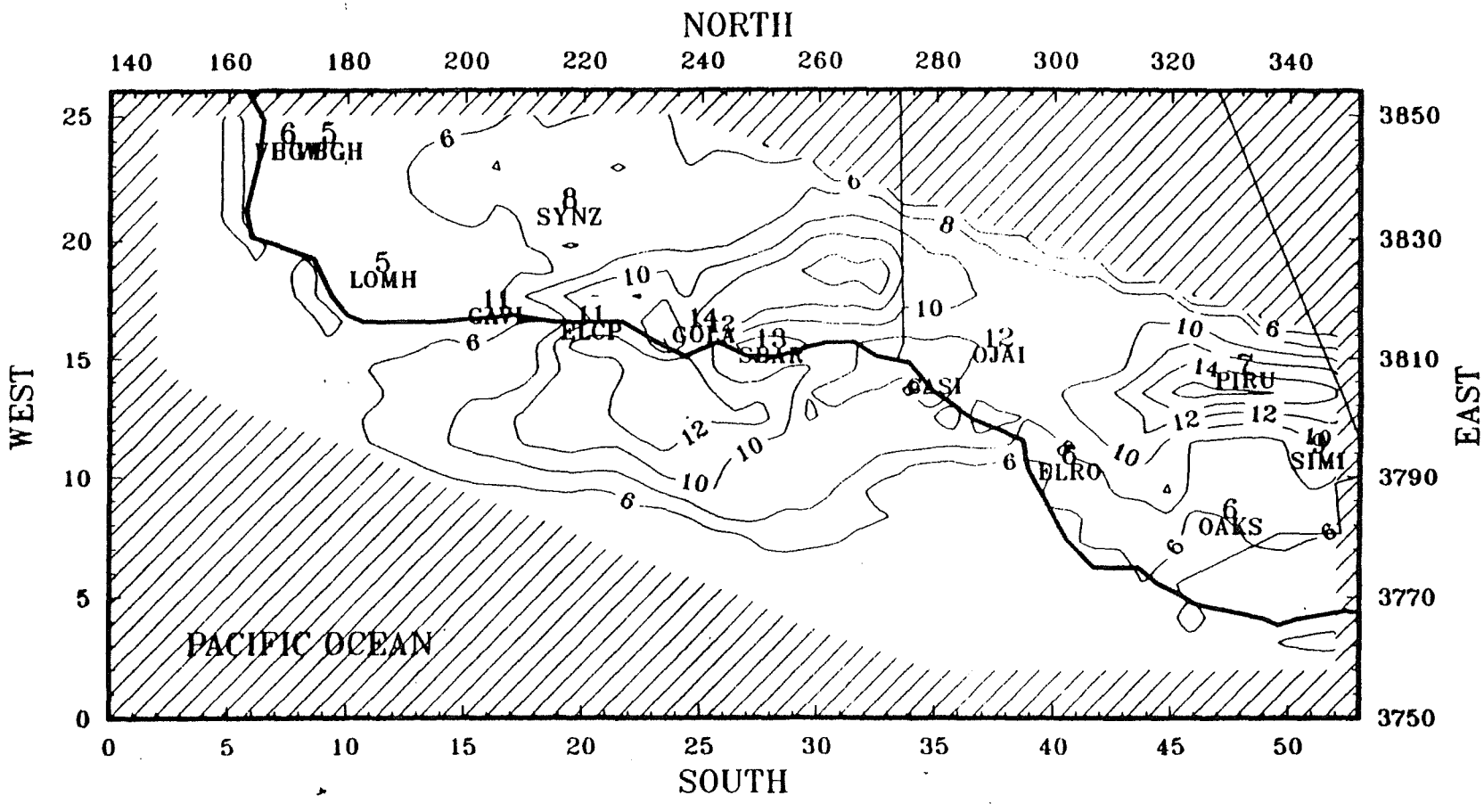
2. COMPARE THE OBSERVATION AT x TO THE PREDICTION AT o_1, o_2, o_3, OR o_4 WHICH IS NEAREST IN VALUE TO THE OBSERVATION AT x

3. COMPARE THE OBSERVATION AT x TO A DISTANCE WEIGHTED INTERPOLATION TO x FROM THE PREDICTIONS AT o_1, o_2, o_3, o_4





Predicted and Observed Hourly Averaged Ozone Concentrations for 6-7 September 1984.

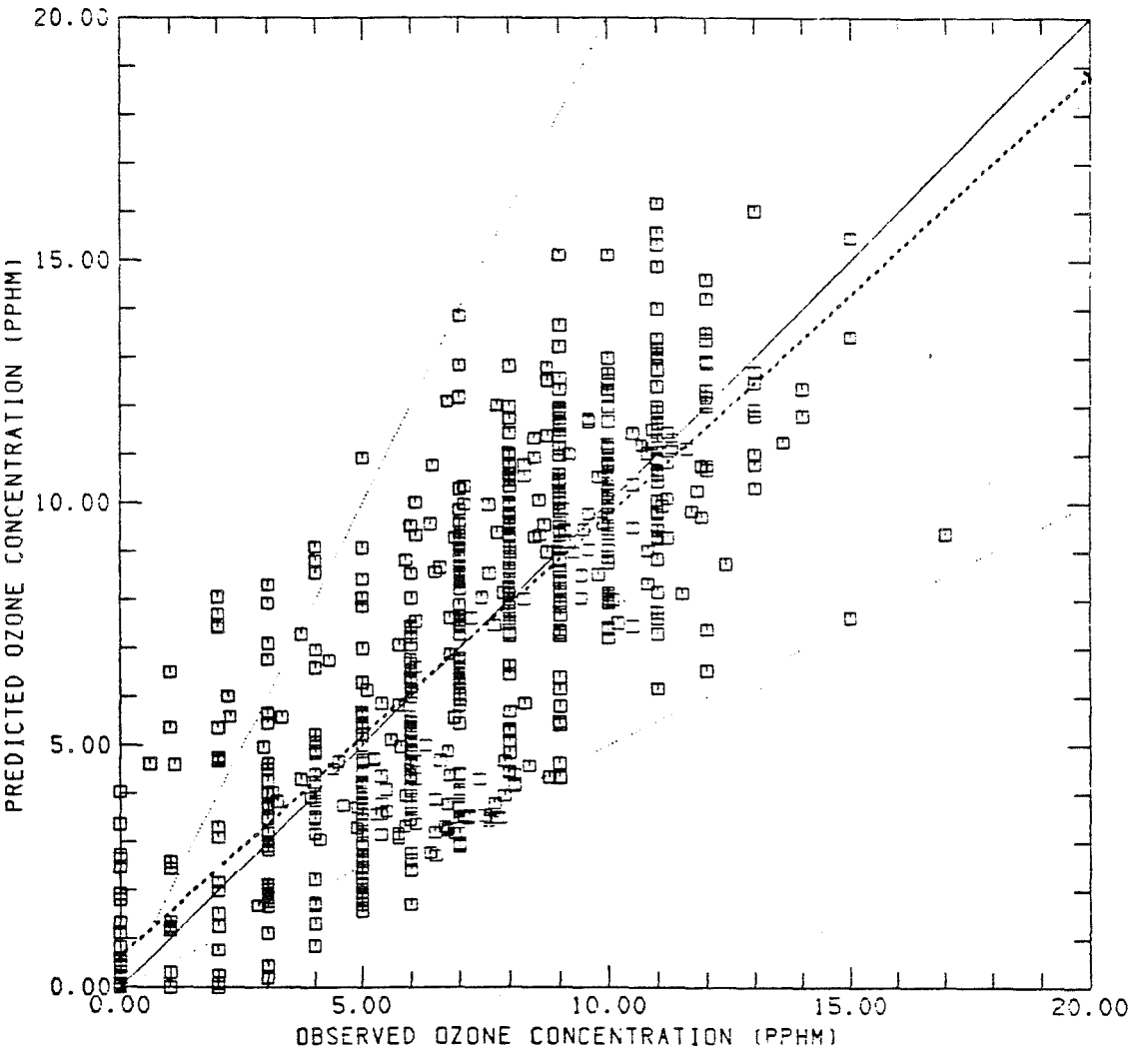


between the hours of 1500 and 1600 PST

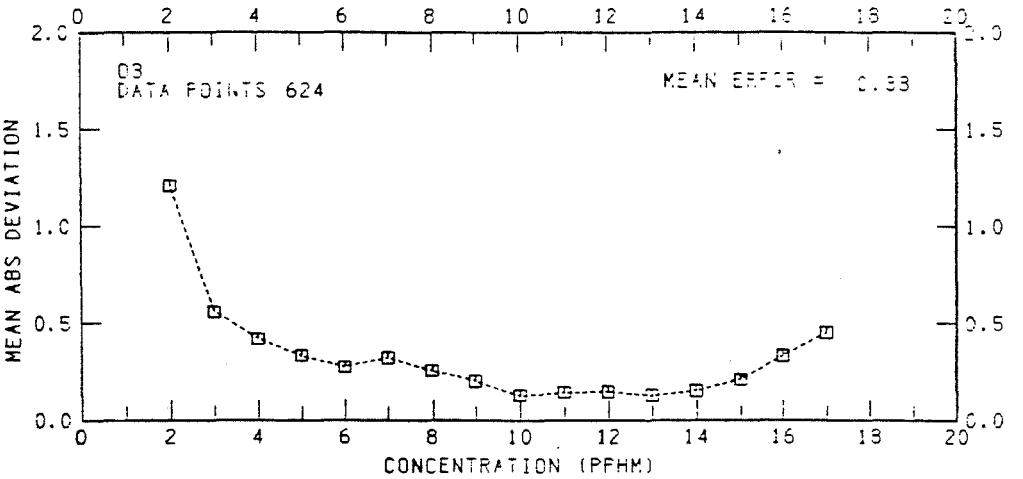
Predicted Ground Level Ozone Concentrations Fields for 7 September 1984.

NUMBER OF POINTS: 663

PERCENT WITHIN FACTOR OF 2 ABOVE 2. PPHM : 88.
SLOPE OF REGRESSION LINE: 0.91
INTERCEPT: 0.64
CORRELATION COEFFICIENT: 0.785



KERN COUNTY AIRSHED, SAI BASE CASE, 8-10 AUGUST 1984



MEAN ABSOLUTE REL. DEVIATION AS A FUNCTION OF CONCENTRATION
KERN COUNTY AIRSHED, SAI BASE CASE, 8-10 AUGUST 1984

PERFORMANCE EVALUATION WITH GRAPHICS

PEAK CONCENTRATIONS: ACCURACY & TIMING

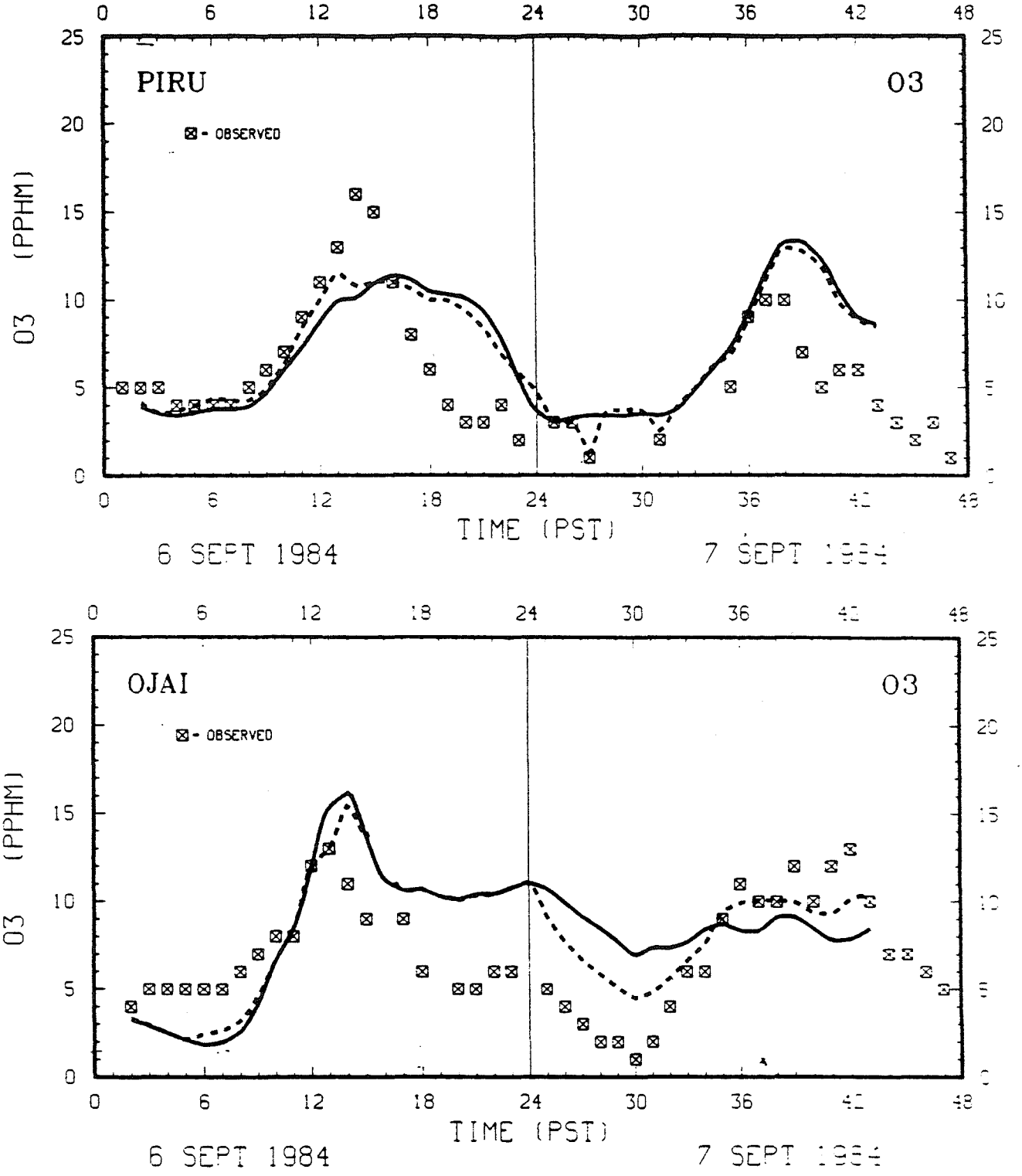
* STATION PLOTS
* ISOPLETH PLOTS

BIAS & ERROR

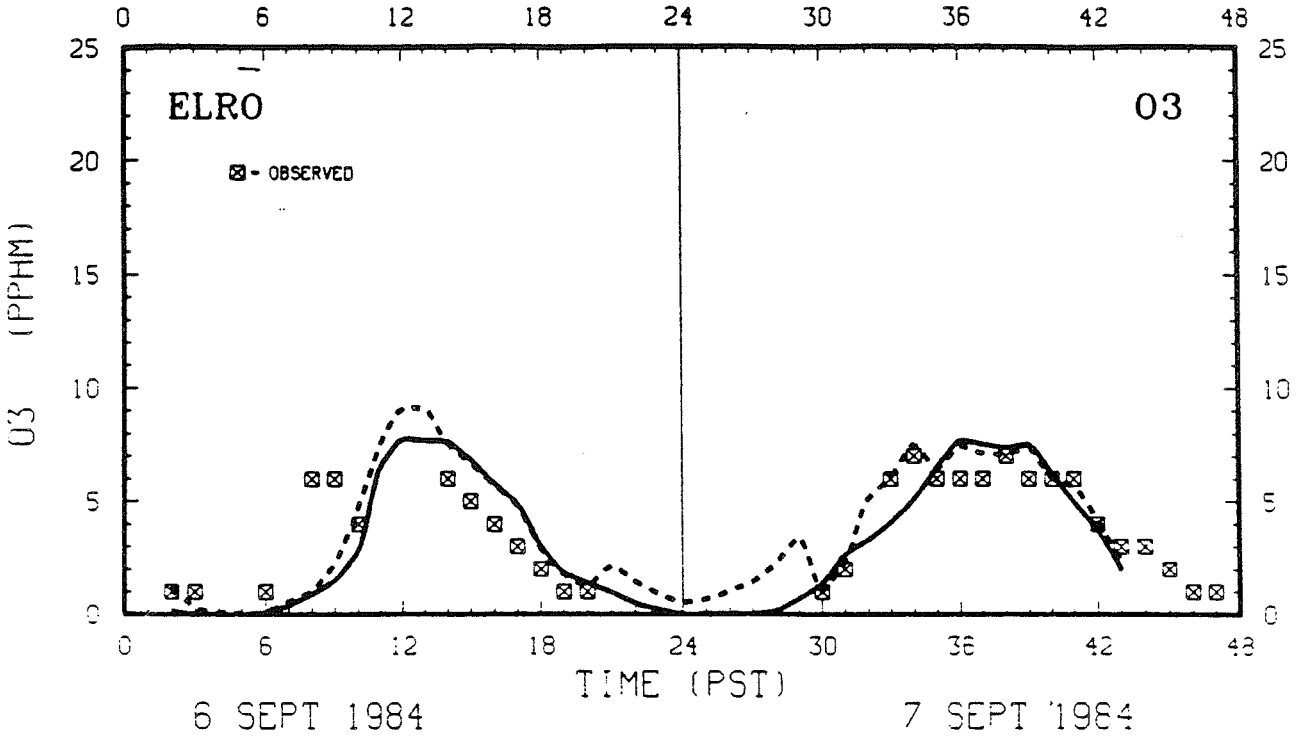
* SCATTER PLOTS
* RESIDUAL PLOTS

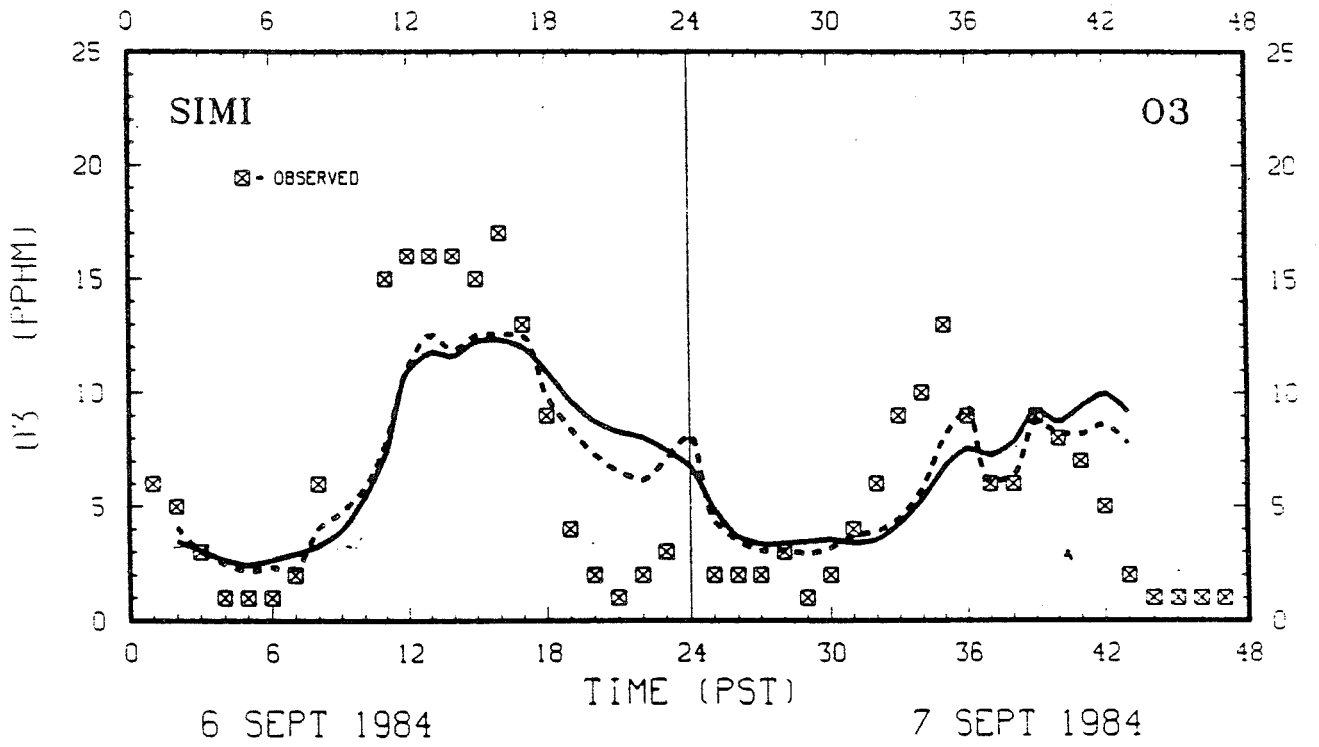
CORRELATION

* STATION PLOTS
* SCATTER PLOTS
* RESIDUAL PLOTS

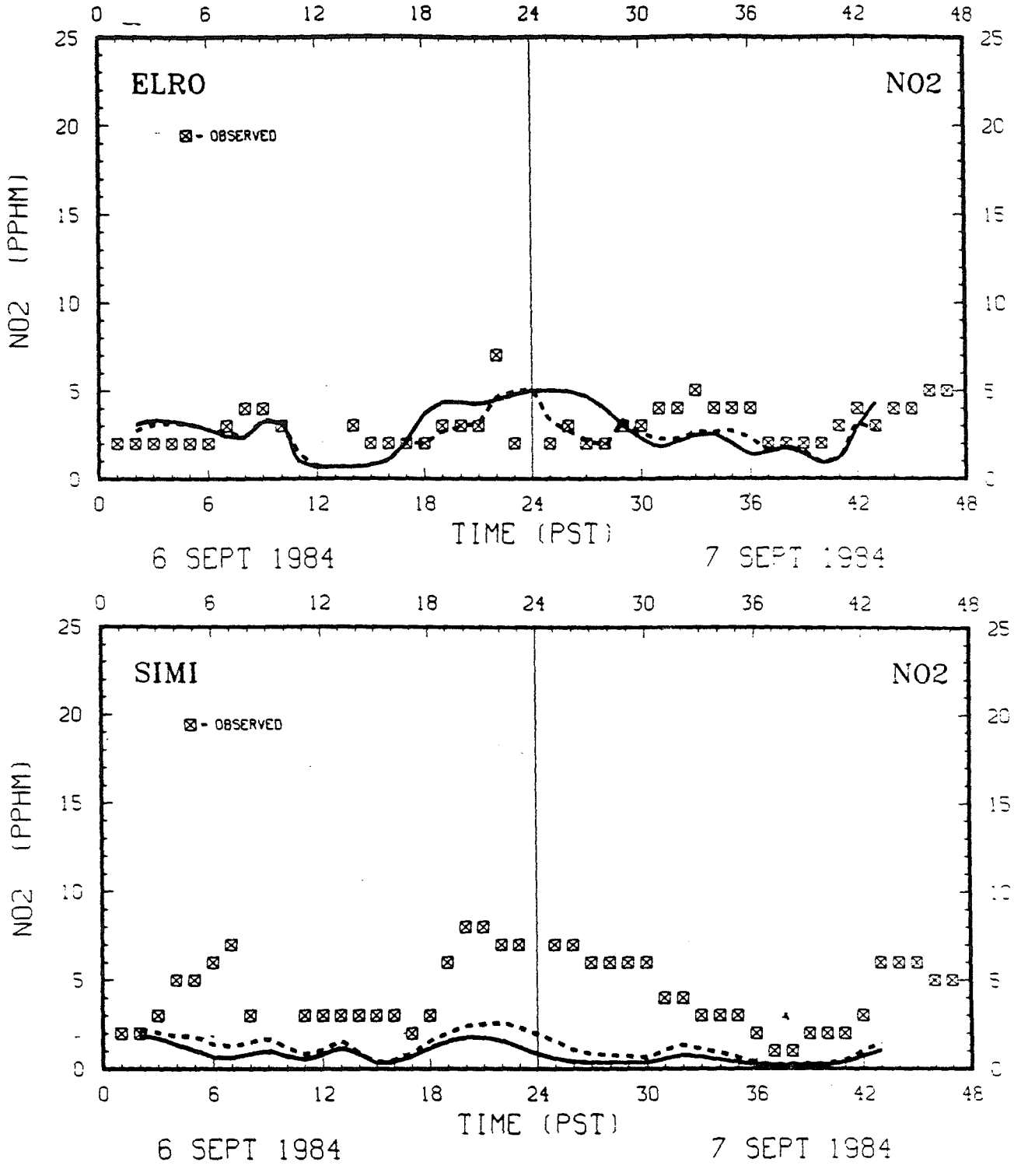


Predicted and Observed Hourly Averaged Ozone Concentrations for 6-7 September 1984.

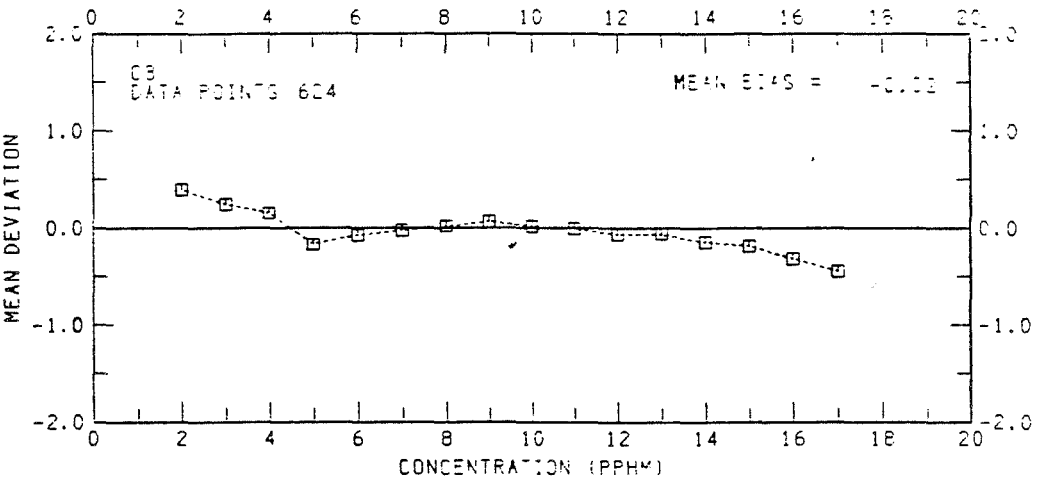




Predicted and Observed Hourly Averaged Ozone Concentrations for 6-7 September 1984.



Predicted and Observed Hourly Averaged NO_2 Concentrations for 6-7 September 1984.



MEAN REL. DEVIATION (PRED - MEAS) AS A FUNCTION OF CONCENTRATION
KERN COUNTY AIRSHED, SAI BASE CASE, 8-10 AUGUST 1984

CONTRIBUTORS TO UNCERTAINTY

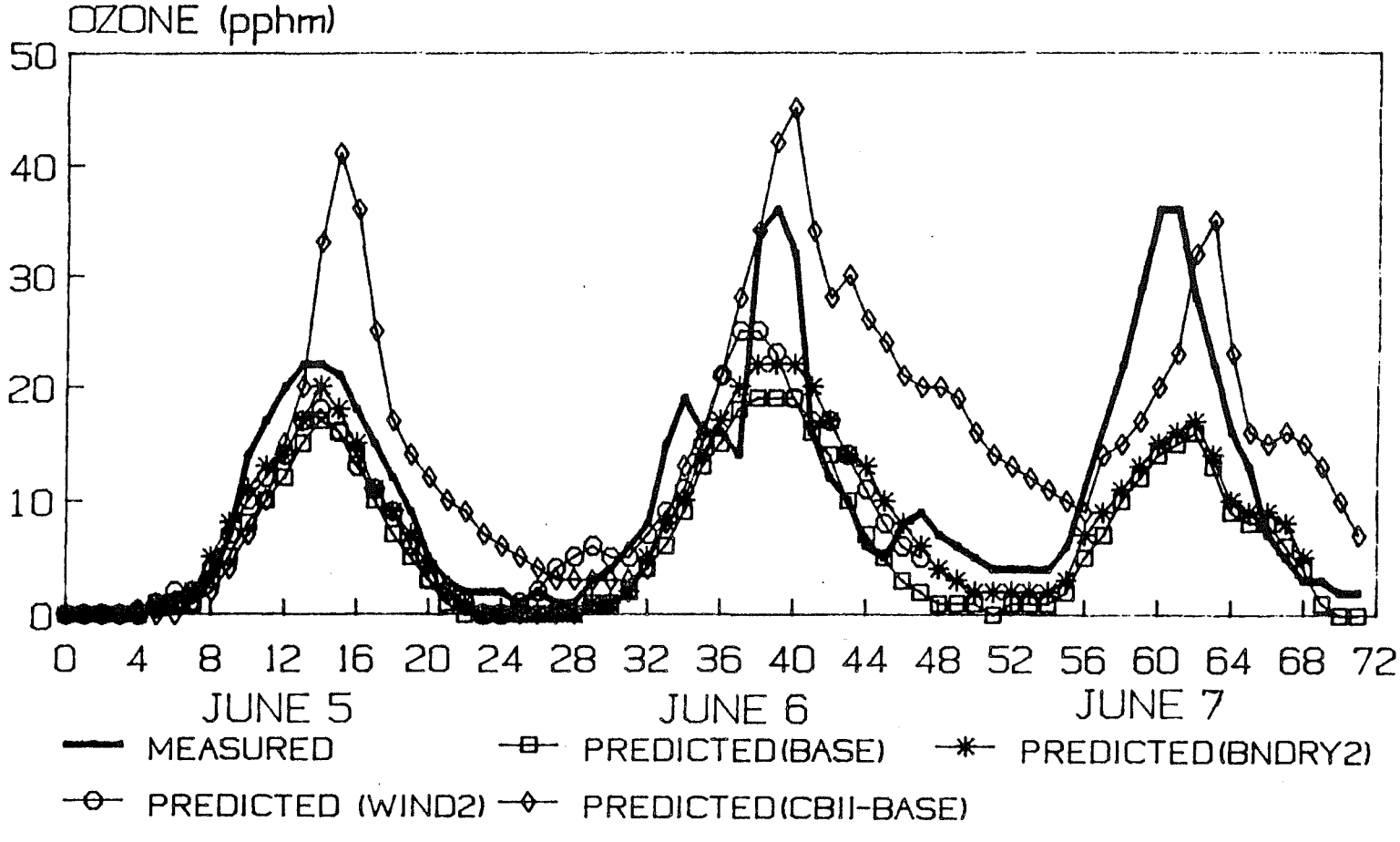
* MODEL FORMULATION

* MODEL INPUTS

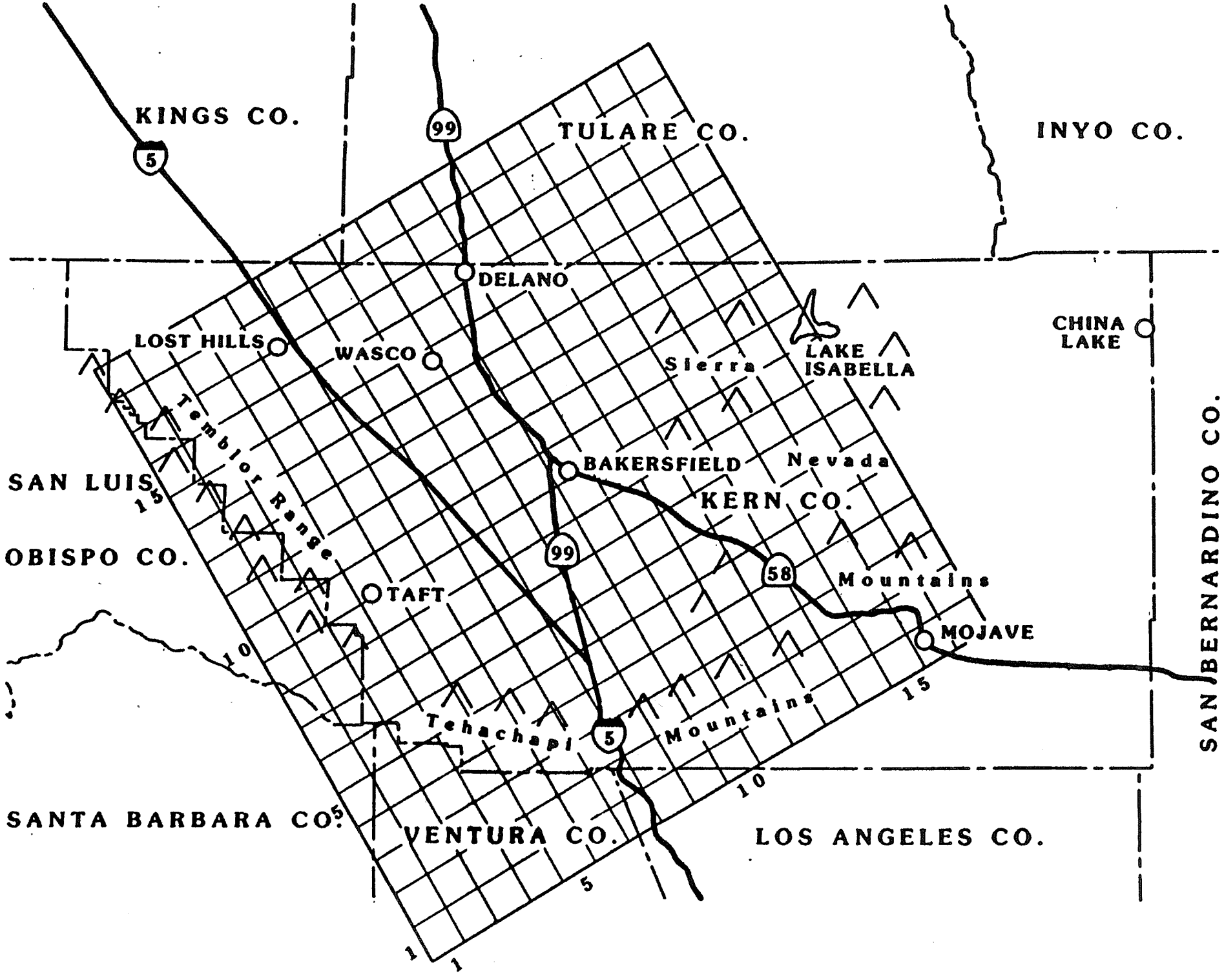
* OBSERVATIONAL UNCERTAINTY

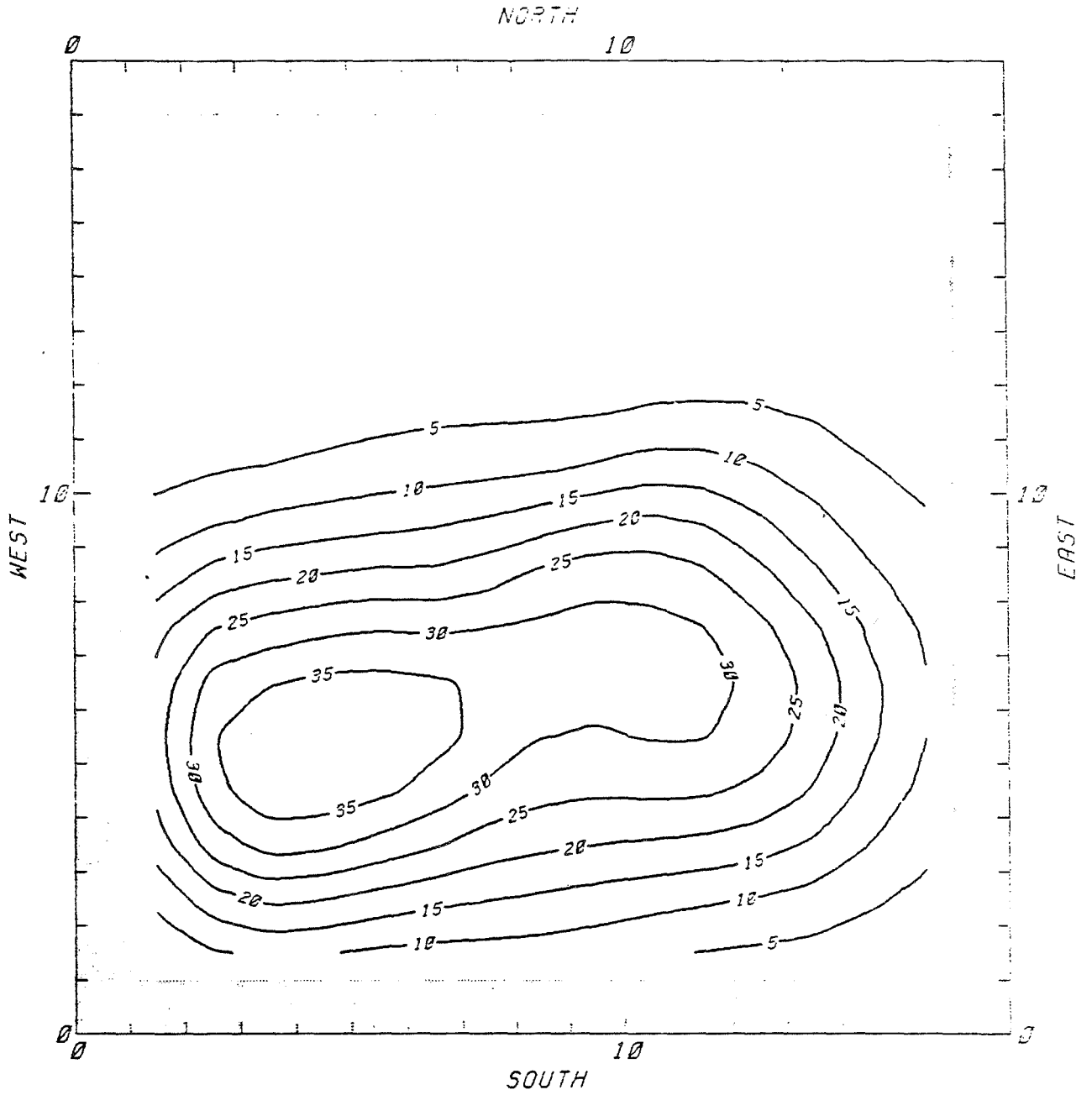
* PREDICTION UNCERTAINTY

COMPARISON OF MEASURED AND PREDICTED OZONE AT GLENDORA JUNE 5-7, 1985

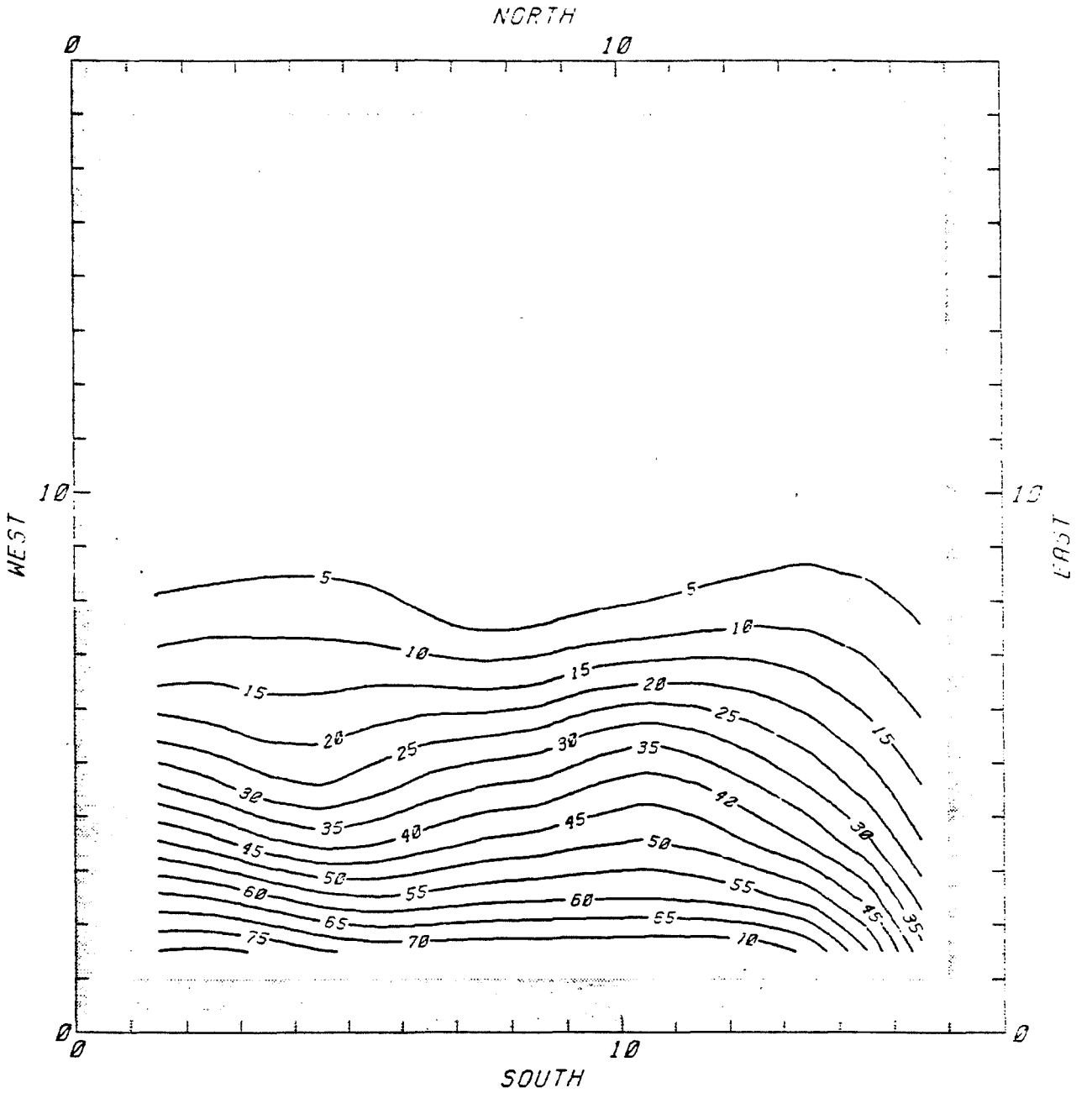


SCE

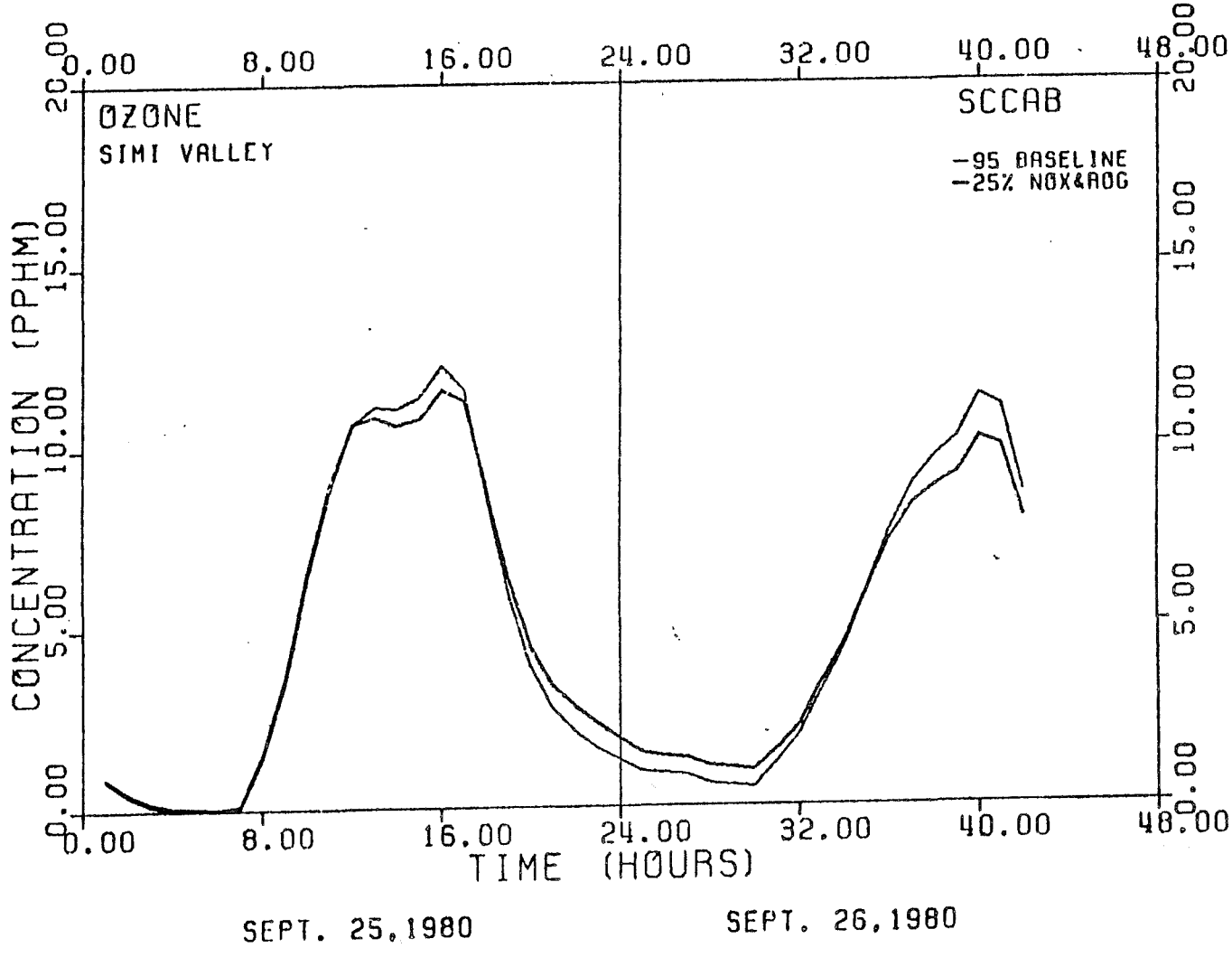

KINGS CO.
TULARE CO.
INYO CO.
DELANO
LOST HILLS
WASCO
Sierra
LAKE ISABELLA
CHINA LAKE
Temblor Range
BAKERSFIELD
Nevada
SAN LUIS OBISPO CO.
KERN CO.
TAFT
Mountains
MOJAVE
SAN BERNARDINO CO.
Tehachapi
Mountains
SANTA BARBARA CO.
VENTURA CO.
LOS ANGELES CO.
99
5
58
15
10
1



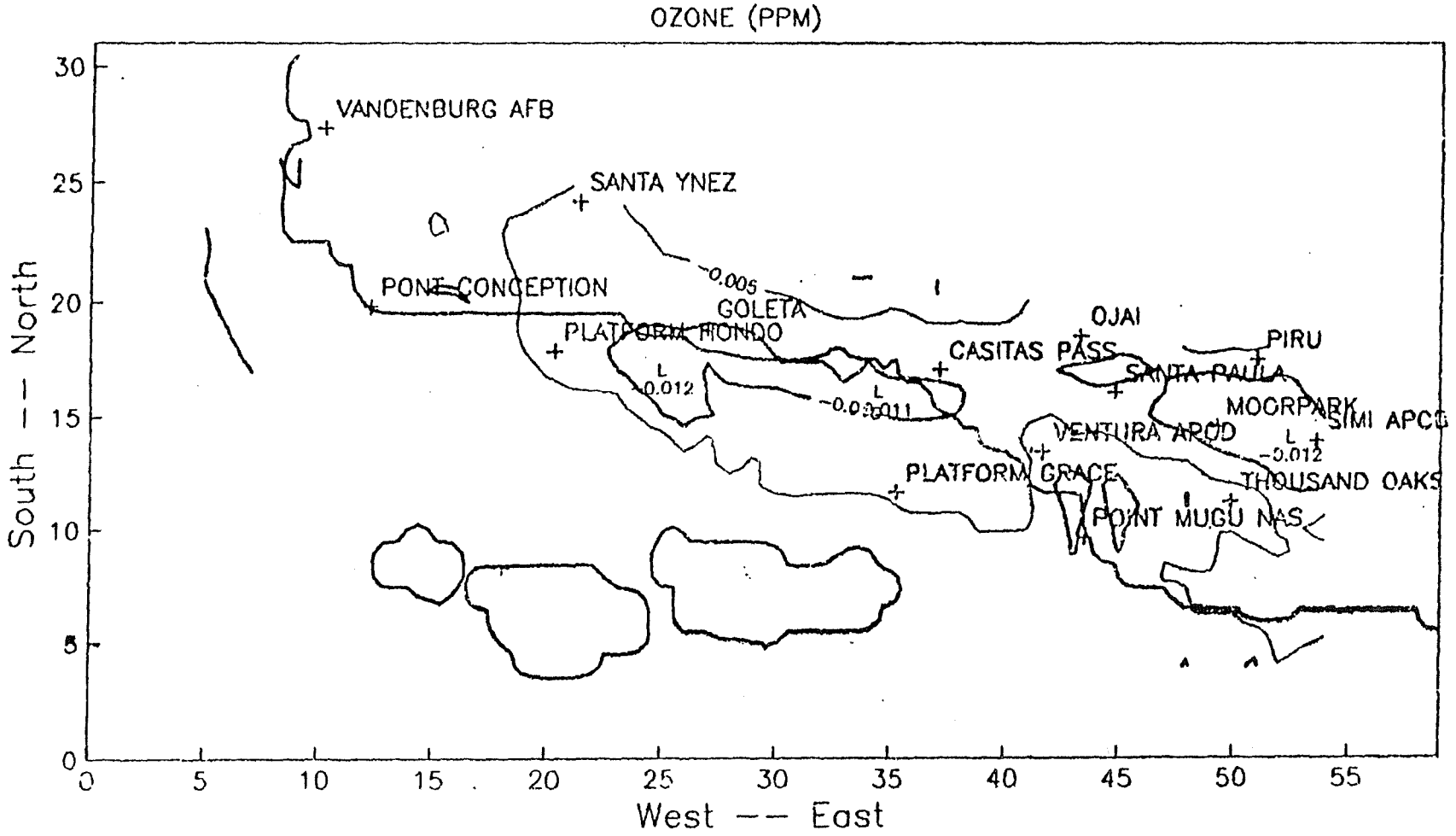
SAI AIRSHED 0000-0200 TRACER CONC FOR AUGUST 7-9 (PPHM)
BETWEEN THE HOURS OF 13 AND 14



SAI AIRSHED INITIAL TRACER CONC FOR AUGUST 7-9 (PPHM)
BETWEEN THE HOURS OF 17 AND 18


OZONE
SIMI VALLEY
SCCAB
-95 BASELINE
-25% NOX&ROG
CONCENTRATION (PPHM)
0.00
5.00
10.00
15.00
20.00
0.00
8.00
16.00
24.00
32.00
40.00
48.00
TIME (HOURS)
SEPT. 25,1980
SEPT. 26,1980

25 Percent NOx and ROG Control Minus 1995 Baseline



MAXIMUM DIFFERENCE BETWEEN HOUR 0 ON SEP 26, 1980 AND HOUR 18 ON SEP 26, 1980 (LEVEL 1)

CURRENT ISSUES

1. Decision makers' limited confidence in models

2. Limited relevance and utility of the results of performance evaluations

3. Lack of standardized, accepted procedures

Area of agreement: Need for improvements in procedures

SUGGESTIONS AND RECOMMENDATIONS

1. Develop tests of model performance that link clearly and directly to the needs of DMs.

2. Analyze field data to identify characteristics that relate to the needs identified.

3. Develop performance tests that are diagnostic in character.

4. Devise tests that stress the model.

PROCESS FOR DEVELOPING DIRECTED TESTS

1. Specify key policy questions.

2. Develop corresponding technical questions.

3. Identify comparisons of particular value in addressing questions posed.

4. Analyze field data to further develop appropriate comparisons.

5. Develop tests.

6. Identify data needed to support tests.

7. Determine if available data are adequate, or if added data should be acquired. Consider costs and benefits.

EXAMPLE -- EVALUATION OF RADM

1. The policy issue -- one of two

   Source attribution

2. Technical question -- one of several

   "How well are transport and rainout represented in RADM?"

3. Result of analyzing field data --

   Correlation of observed precipitation with wet deposition, but not with concentration of gaseous pollutants.

4. Tests --

   Compare observed precipitation with predicted concentrations; with predicted deposition.

EXAMPLE --
TESTING A MODEL OVER A RANGE OF CONDITIONS

1. Retrospective or historical comparisons.

   1975 base case; 1985 emissions.
   Compare for 1985.

2. Comparisons for a range of adverse conditions.

   For SOCAB - SCAQMD and SCE
   Episodes selected from four categories of meteorology.

3. Study of "non-adverse" days as well.

4. Study of similar meteorologies in different areas of CA, using the same model. Different emissions rates and patterns.

5. Carry out corroborative analyses.

6. Develop a protocol for model evaluation.

7. Institute an "open process" for performance evaluation.

8. Revise the "model" of model development - from product to process.

9. Integrate planning for modeling and data collection.

PROPOSED ACTIONS

1. Adopt suitable time scales for action.

2. Develop NRC-type scoping paper.

3. Commit funding for the longer term.

4. Carry out R & D in timely and responsive manner.

5. Apply new procedures ASAP, to test them.

6. Set up a forum for interaction between the technical and policy communities.

7. Develop a scoping of data needs.

8. Define and fund corroborative analysis efforts.

9. Introduce procedures in ARB guidelines on continuing basis.

THE ROLE OF DIAGNOSTIC ANALYSIS IN PHOTOCHEMICAL MODELING

KEY QUESTIONS:

- Where do models derive their credibility?
- What is diagnostic analysis?
- Why is it needed?
- How should it be performed?

RELATED TOPICS:

- Input parameter uncertainty
- Model uncertainty
- Sensitivity analysis
- Optimization of model performance

MODEL CREDIBILITY

MODEL FORMULATION:

- Acceptance by technical experts
- Acceptance by regulatory agencies
- Continual updating to incorporate best science

MODEL INPUT DATA:

- Is aerometric data base sufficient to run the model?
- Are the inputs for uncertain parameters consistent with available data?

MODEL CREDIBILITY

MODEL TESTING:

- Model Performance Evaluations
  - Are bias and error small?
  - Is the bias systematic or random?
- Model Sensitivity Analysis
  - Is it sensitive to the expected parameters?
  - Is it highly sensitive to unknown parameters?
- Model Performance for Emission Change Experiments
  - Smog chamber experiments
  - Future model evaluations

What is Diagnostic Analysis?

- The process of objectively selecting values of uncertain model inputs to maximize model credibility
- Exploring model sensitivity to plausible input parameter variations
- Optimization of model performance with constraints on acceptable parameter values
- Familiarity with the aerometric data base and general relationships in the model is essential

Why is Diagnostic Analysis Performed

- Models are imperfect
  - Model formulation is simplified
  - Chemical mechanism is accurate to only 20-25%
  - Transport and dispersion idealized
- Aerometric data base is sparse and uncertain
  - Measurement error is typically 5-10%
  - Data representativeness is uncertain

  Emissions data may have 20-30% uncertainty
- The available data must be extensively interpolated and extrapolated to generate model inputs
- Diagnostic analysis is needed to select the best inputs and understand the limitations of the model results

How Should Diagnostic Analysis be Performed

- The approach should be described in the modeling protocol

- No one approach is suitable for all situations

- The approach will depend on a number of factors:

  - Nature of the air quality problem
    - Local ozone generation
    - Transport dominated ozone problem

  - Aerometric data base
    - Extent
    - Uncertainty
    - Are critical parameters missing?

  - Complexity of the meteorology
    - Single day simulations of well developed flow
    - Multi-day simulations of complex flows

  - Type of wind field model
    - Diagnostic
    - Prognostic

The Photochemical Modeling Protocol

- Model selection
- Emissions data base selection
- Analysis of the meteorology and and air quality data
- Selection of the ozone episodes
- Parameter variations for diagnostic analysis
- Base case selection procedures
- Model performance acceptance criteria
- Future emission scenarios
- Sensitivity analysis for runs with future emissions

How Sparse is the Modeling Data Base?

Consider:

- Grid model application
- Special study data base
- Grid of 25 x 25 x 5 cells
- 20 surface wind stations
- 20 air quality stations
- 4 upper air met stations (4 soundings per day)
- Intermittent air craft data

Wind Fields:

- Model requires 75,000 wind inputs per day
- Data availability
  - -544 wind observations per day
  - -1 out of 31 suface cells every hour
  - -1 out of 156 elevated cells every 6th hour

How Sparse is the Modeling Data Base?

Mixing Heights:

- Model requires 15,000 inputs per day
- Data base provides 16 to 30 observations per day

Temperature and Relative Humidity:

- Sparseness comparable to wind data

Inflow Boundary Concentration:

- Model requires 6,000 inputs per species per day
- Data for 1 out of 25 surface cells
- Data for 1 out of 120 elevated cells

Initial Concentrations:

- Model requires 3125 concentrations per species
- Data for 1 out of 30 surface cells
- Data for 1 out of 600 elevated cells

How Uncertain are the Emissions?

Man-made mobile emissions:

- VMT and trips
- VMT mix - fleet composition
- Control system deterioration rates
- Composite emissions factors

Man-made Stationary Emissions:

- Major sources
- Minor sources

Natural Emissions:

- Biomass amounts
- Vegetation emissions factors
- Natural seep emissions

Speciation of Organic Emissions

What Parameters should be Adjusted?

CONSIDER ADJUSTING:

- Natural emissions
- Mixing heights
- Winds aloft
- Initial concentrations
- Boundary concentrations
- Dry deposition resistance

AVOID ADJUSTING:

- Man-made emissions
- Chemical mechanism
- Surface winds
- Atmospheric stability

How Much Discretion Should be Given to Modelers?

- Modelers can be trusted
- Make modeling an open process
- Specify diagnostic analysis runs in protocol
- Modelers need the discretion to make additional runs that they believe could be important

APPLICATION OF URBAN AIRSHED MODEL FOR REGULATORY ANALYSIS IN THE SOUTH COAST AIR BASIN

Planning Division
South Coast Air Quality Management District
June, 1986

I. INTRODUCTION

District contracted with Systems Applications, Incorporated (SAI) to conduct a number of Urban Airshed Model (UAM) simulations to address the following three questions related to ozone air quality:

1) The sensitivity of the model to nighttime chemistry

2) The effect of various transfers of emissions between the eastern and western portions of the Basin (East/West Tradeoff)

3) The effect of 0.4 grams/mile NO_x Control Program

This staff report documents the model runs and the modeling results.

I.1 Model Sensitivity to Nighttime Chemistry

Previous UAM applications in the South Coast Air Basin by SAI did not address the nighttime chemistry associated with nitric acid formation. Significant nitric acid can form at night via reactions involving NO_3 and N_2O_5. The conclusions of these modeling analysis have been questioned because the nighttime chemistry was not included in the chemical mechanism of the UAM. Therefore, it is very important to determine the sensitivity of the model predictions on the inclusion of the nighttime chemistry in the overnight episodic simulation.

The most important reactions occurred in the night are as follows:

$$NO + O_3 \rightarrow NO_2 + O_2$$

$$NO_2 + O_3 \rightarrow NO_3 + O_2$$

$$NO_3 + NO_2 \rightleftharpoons N_2O_5$$

$$NO_3 + NO_2 \rightarrow NO + NO_2 + O_2$$

$$N_2O_5 + 2H_2O \rightarrow 2HNO_3$$

Because these reactions effectively provide a sink for NO in the night, there will be less NO available for ozone scavenging in the next morning. The inclusion of nighttime chemistry is directionally likely to increase the potential for higher ozone concentrations in the coastal and central portions of the Basin and to increase the potential impact of fresh NOx emissions to the ozone concentrations.

I.2 East-West Emission Trade-Off

District Rule 1307 requires stationary sources to offset emission increases by an offset factor determined as follows:

Offset Factor = 1.1 + bx

where: b = 0 when x is less than eight kilometers
b = 0.01 when x is equal to or greater than eight kilometers

x = the distance between the affected source permit unit and the offset source permit unit (in kilometer)

This calculated Offset Factor shall not exceed 1.5.

Most of the existing sources of emissions with the potential to be relocated (either by emissions trading or physical relocation of the facility) are located in the coastal and central portions of the Basin. Under existing District Rules, new sources located in the inland counties are most likely required to secure trade-off at a higher offset ratio than new sources seeking to locate in the western and central portions of the Basin. Various Rule revisions have been suggested which would modify the offset factor calculation. The UAM was used to examine if there are air quality impacts associated with these alternatives. A number of model simulations were conducted to provide information on the Basinwide ozone improvement/deterioration of shifting ROG and NOx emissions from the coastal and central portions of the Basin to the inland area.

I.3 0.4 gram/mile NOx Control Program

ARB has newly adopted the 0.4 gram/mile NOx emission standard for light-duty vehicles to be implemented in 1994. Because of the large reduction of NOx emissions projected for this control measure, it is of interest to determine the Basinwide ozone impacts of implementing this measure.

II. BACKGROUND

The UAM developed by SAI is a grid-based physiochemical model which is well suited for predicting spatial and temporal distribution of photochemical pollutant concentrations in an urbanized area. It includes state-of-the-art treatments of atmospheric chemistry, advective transport, turbulent diffusion, surface removal, microscale phenomena, and mass conservation. This model has been validated against the June 26-27, 1974 ozone episode and the November 7-8, 1978 NO_2 episode in the South Coast Air Basin. A number of large-scale UAM simulation studies have been conducted for the Basin in the past five years. It is the only regional gridded photochemical dispersion model recommended by EPA for regulatory use in regional ozone air quality analysis.

The June 26-27, 1974 meteorological conditions was used in all UAM simulations reported here. It is an episode with high ozone formation potential. The emission input data represents situations likely to occur in the year 2000 including reductions from controls applied on existing sources of emissions. The 2000 Basinwide NOx emissions are 847 tons per day and for ROG are 792 tons per day. About 60 percent of the emissions for both NOx and ROG are from mobile sources. All emission changes are applied to mobile source emissions in all the simulations conducted because it is the easiest way to make significant changes of Basinwide emission.

III. MODELING ANALYSIS

Table III-1 lists all the modeling scenarios of this UAM study. The scenario denoted X_1 is a modeling run conducted by SAI for the Western Oil and Gas Association (WOGA) for a 1987 emission scenario with the most emissions reductions. It approximates the projected emissions for NOx and ROG for the year 2000 with all foreseeable controls. Figure III-1 displays the UAM modeling region and the arbitrarily defined "West" and "East" zones where the assumed emission increases/decreases/shifts would occur as specified in Table III-1.

The differences of model predictions between scenarios S_1 and X_1 displays the sensitivity of including the nighttime chemistry in the Carbon Bond Mechanism (CBM); the chemical mechanism used in UAM. Scenario S_1 is used as the base case (see Section II for base case description) and the differences of ozone predictions between all other individual scenarios and scenario S_1 displays the impacts of specific emission changes associated with specific scenario.

Figure III-2 displays the peak ozone concentration prediction on the second day of the two-day simulation in this Basin for scenario S_1. It is clear that the peak ozone concentrations occurred in the inland areas and the coastal areas would have peak ozone concentrations close or below the federal standard of 12 pphm. The Basinwide peak ozone concentration occurred at Fontana with a value slightly higher than 24 pphm.

III.1 Treatment of Nighttime Chemistry

Figure III-3 displays the changes of peak ozone concentrations by including the nighttime chemistry into the CBM of the UAM. Without nighttime chemistry peak ozone concentrations were underestimated by up to 0.3 pphm in east San Gabriel Valley and in Orange County and overestimated by up to 0.7 pphm in the inland areas. These changes of peak ozone concentrations are consistent directionally with the hypothesis that (1) less NOx will be available for ozone scavenging with the nighttime chemistry and, therefore, earlier build-up of ozone and, (2) less NOx would be available for Basinwide peak ozone formation later on the day.

The changes of peak ozone concentrations in this Basin by including nighttime chemistry (as shown in Figure III-3) are, directionally, similar to those caused by having additional NOx control. Hence, one might expect that the effect of NOx control on peak ozone concentrations would be more pronounced with the inclusion of nighttime chemistry. However, the magnitude of changes as shown in Figure III-3 indicate that there would be no significant influences/changes on the control policy implications derived from previous UAM runs with the inclusion of nighttime chemistry.

III.2 East-West Emission Trade-Off

Figures III-4 to III-7 display the changes of Basinwide peak ozone concentration predictions resulting from changes in NOx and ROG emission as specified under scenarios S_2, S_3, S_4, and S_5, respectively (see Table III-1). These modeling results can be summarized as follows:

TABLE III-1
DESCRIPTION OF AIRSHED MODELING SCENARIOS RELATED TO EAST-WEST TRADEOFF

ID	DESCRIPTION	NOx*	ROG*
X_1	Base Case without Nighttime Chemistry	847 tons/day in the Basin	792 tons/day in the Basin
S_1	Base Case with Nighttime Chemistry	Same as in X_1	Same as in X_1
S_2	1:1 Tradeoff for Both NOx and ROG	128 tons/day Shift from West to East	100 tons/day Shift from West to East
S_3	1:1 Tradeoff between NOx and ROG	100 tons/day Increase in the East	100 tons/day Reduction in the West
S_4	1:1 Tradeoff for ROG	No Change from Base Case	100 tons/day Shift from West to East
S_5	1:1 Tradeoff for NOx with Additonal 1:0.5 Reduction for ROG	100 tons/day Shift from West to East	50 tons/day Reduction in the West
S_6	0.4 g/mile Program with Concurrent ROG Reduction	73 tons/day reduction across the Basin.	85 tons/day Reduction across the Basin

*See Figure 1 for the geographical areas defining "East" and "West". All emission changes were applied on mobile source emissions.

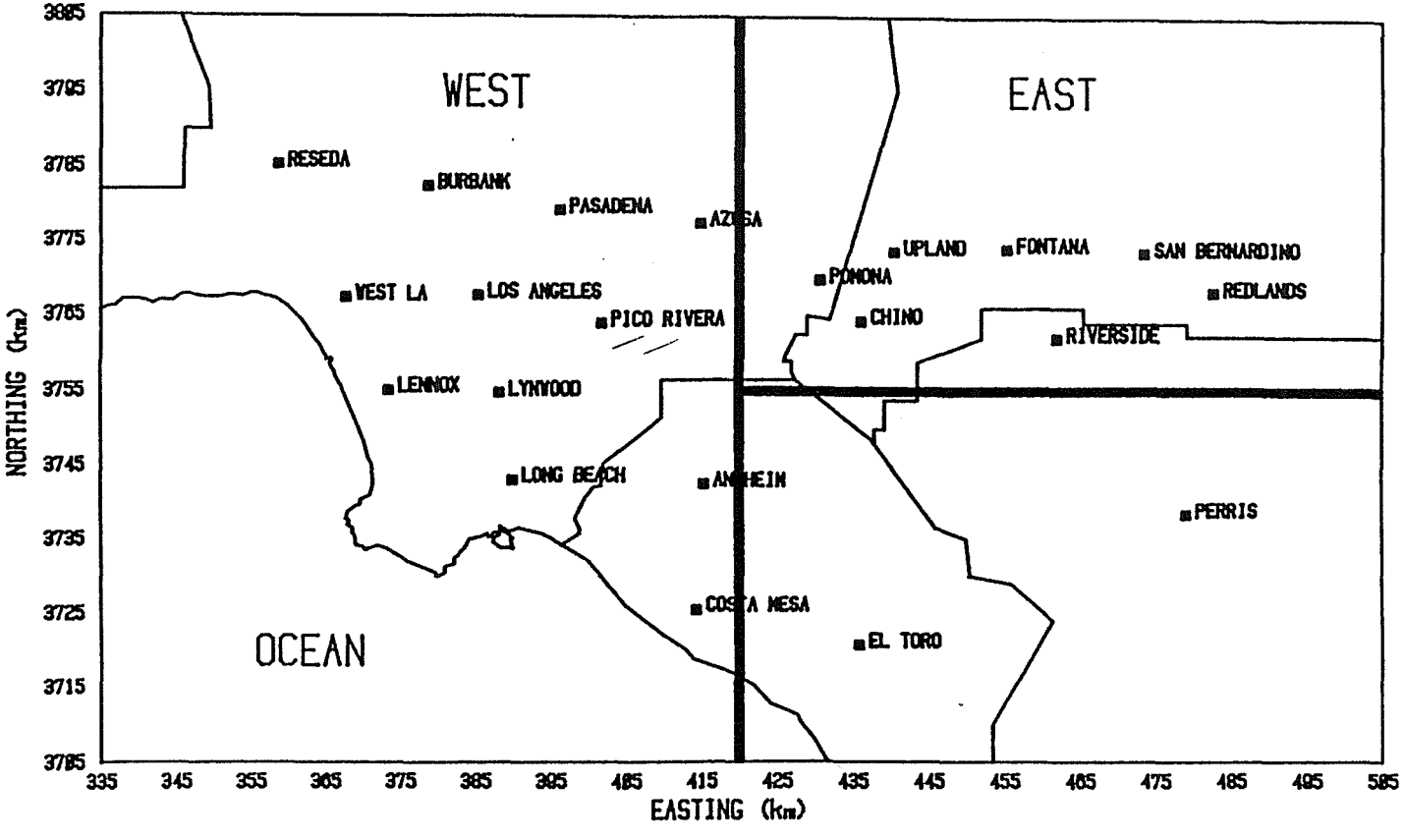


FIGURE III-1
EAST-WEST EMISSIONS TRADEOFF AIRSHED MODELING REGION

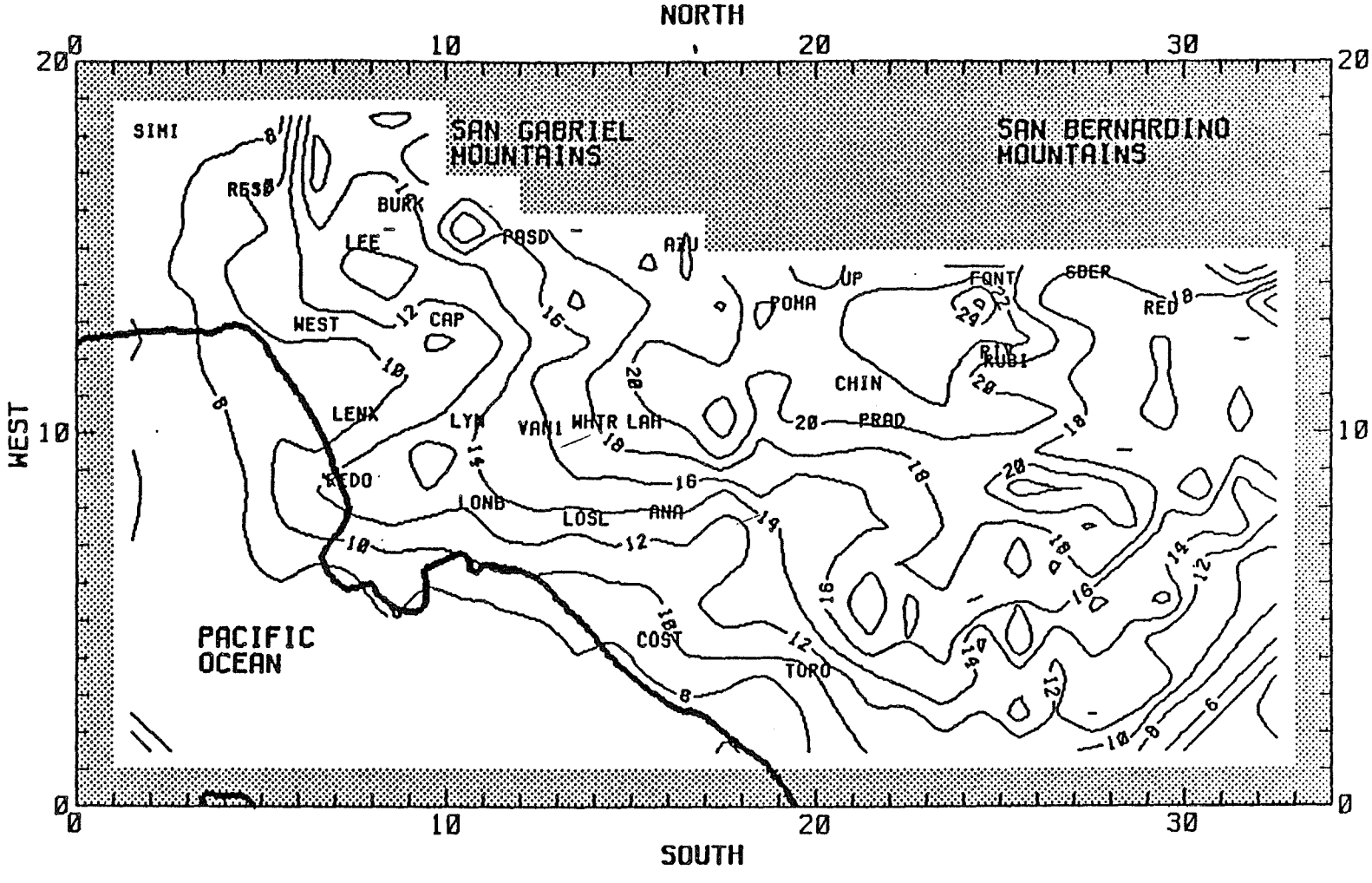


FIGURE III-2

BASE CASE PEAK OZONE CONCENTRATION ESTIMATES (CASE S1)

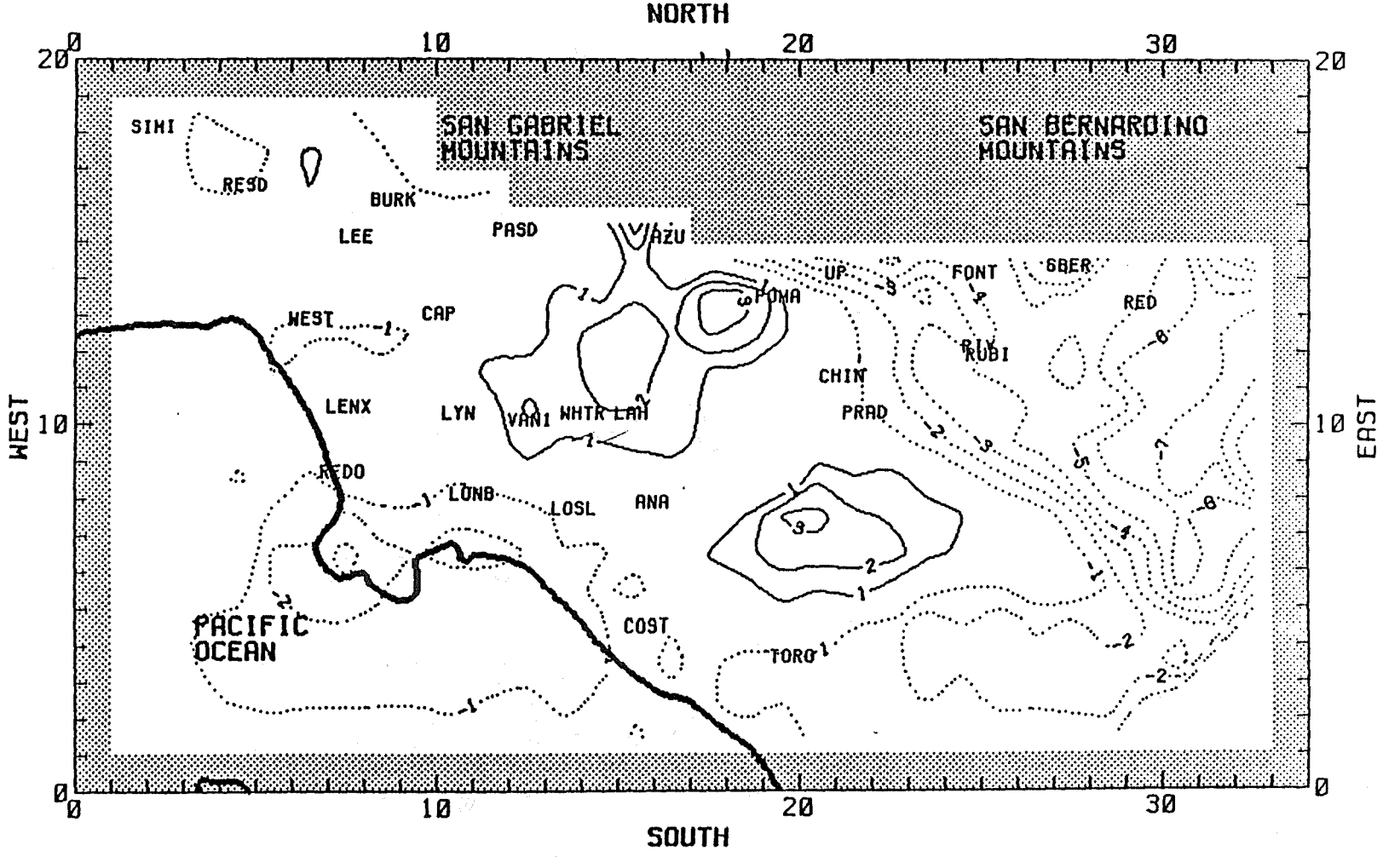


FIGURE III-3
PEAK OZONE CHANGES DUE TO INCLUDING/EXCLUDING NIGHTTIME CHEMISTRY
(CASE S1 - CASE X1)

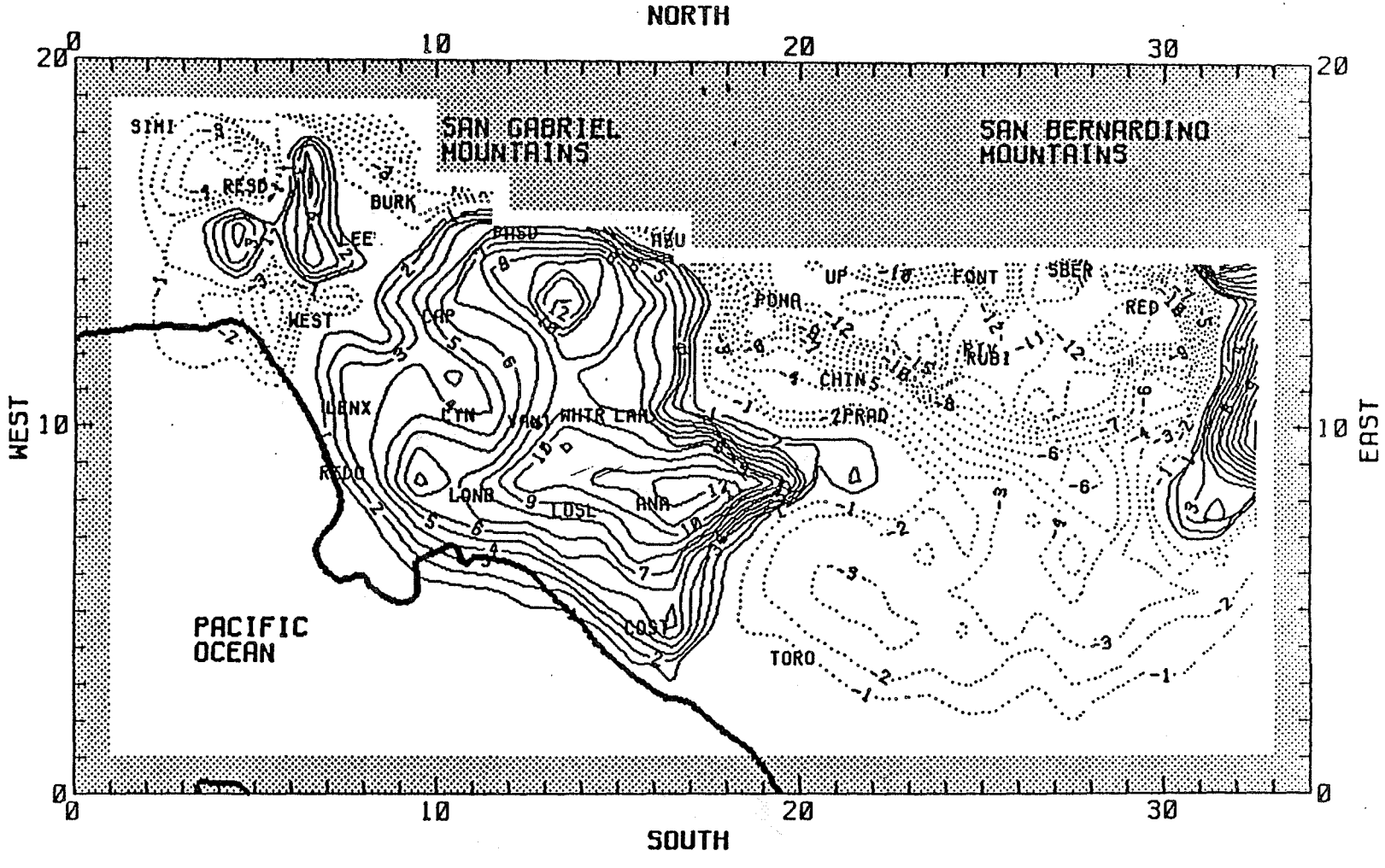


FIGURE III-4

PEAK OZONE CHANGES DUE TO EAST-WEST TRADEOFF FOR BOTH NOX & ROG
(CASE S2 - CASE S1)

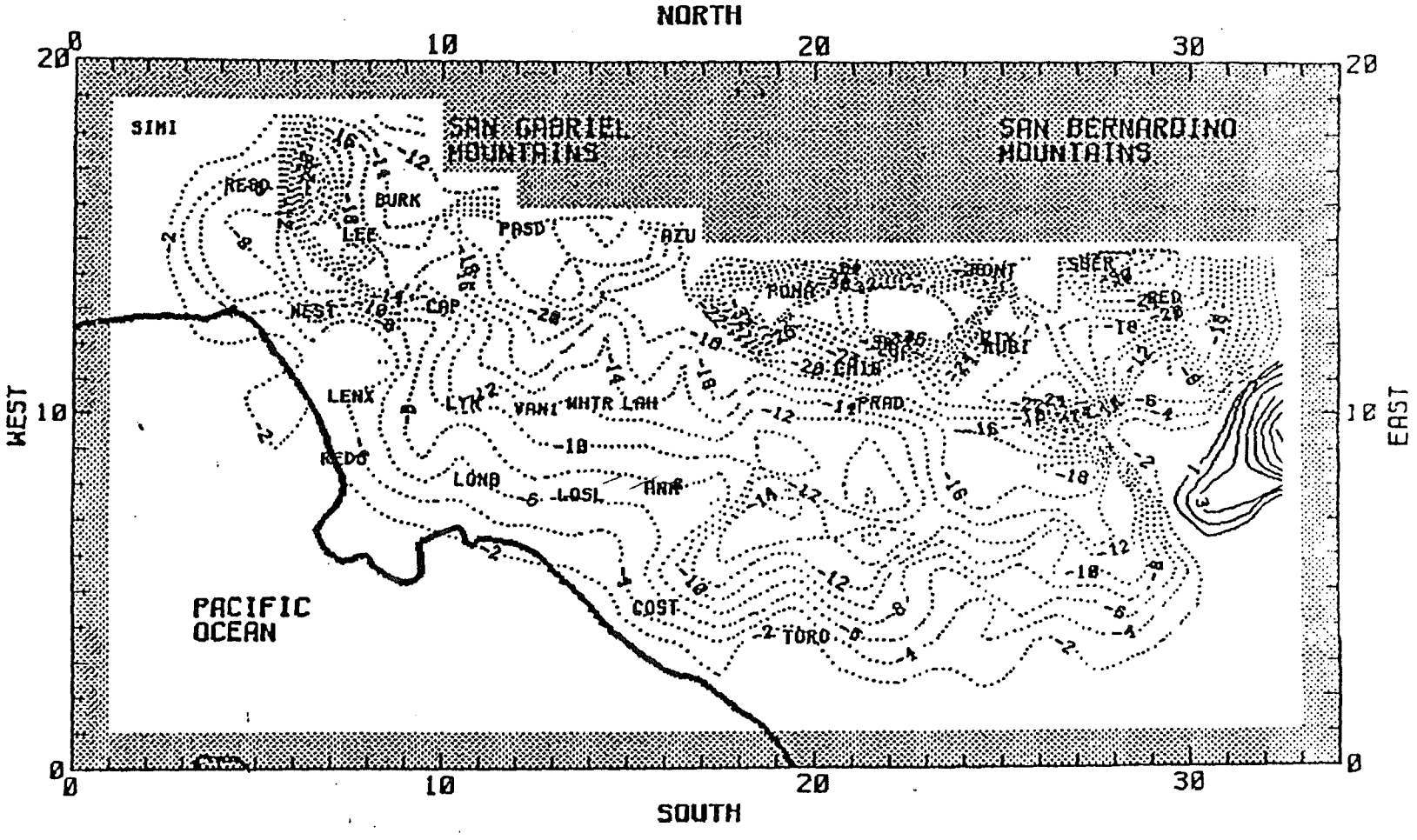


FIGURE III-5
PEAK OZONE CHANGES DUE TO EAST-WEST TRADEOFF BETWEEN NOx and ROG
(CASE S3 - CASE S1)

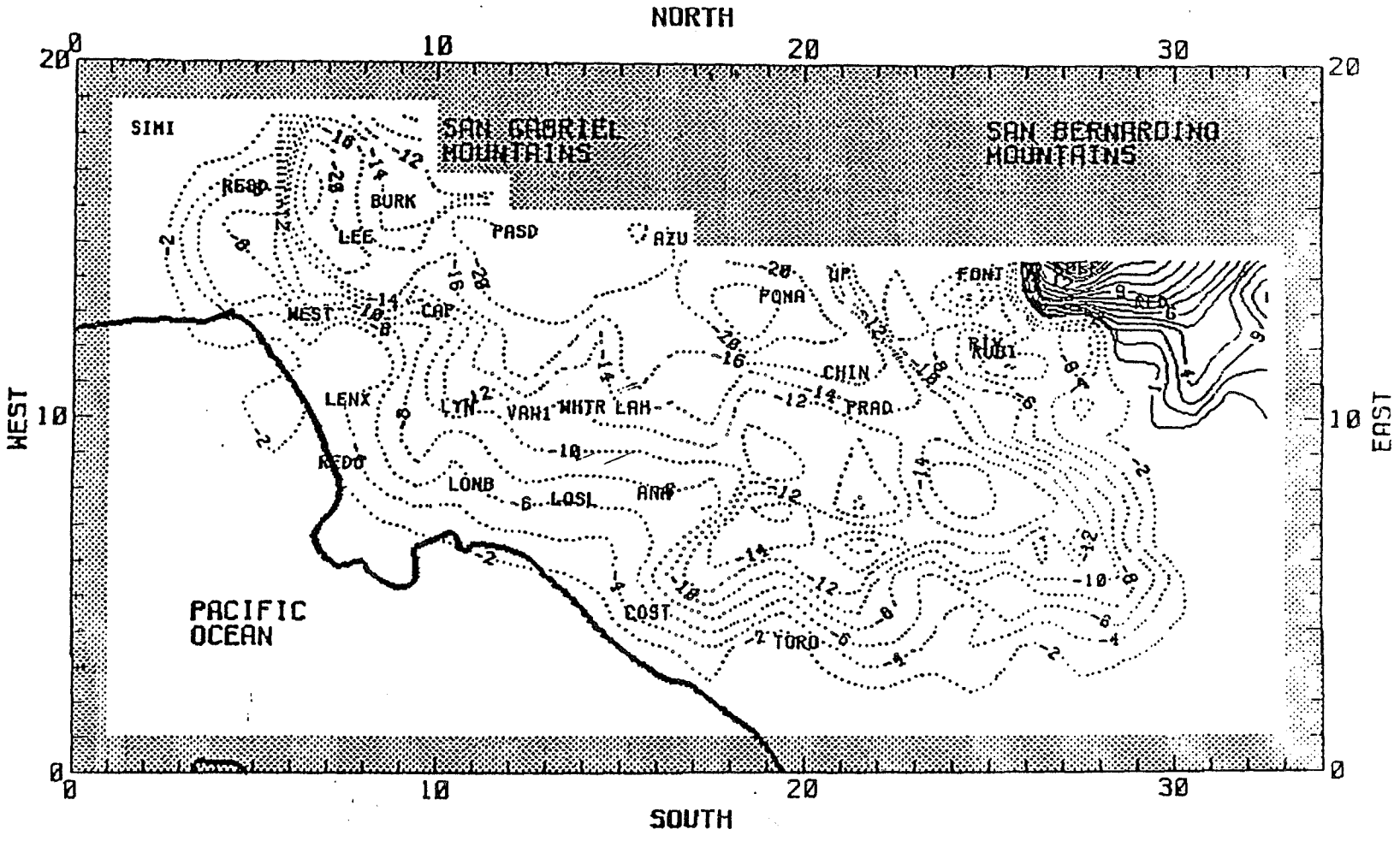


FIGURE III-6

PEAK OZONE CHANGES DUE TO EAST-WEST TRADEOFF FOR ROG EMISSIONS
(CASE S4 - CASE S1)

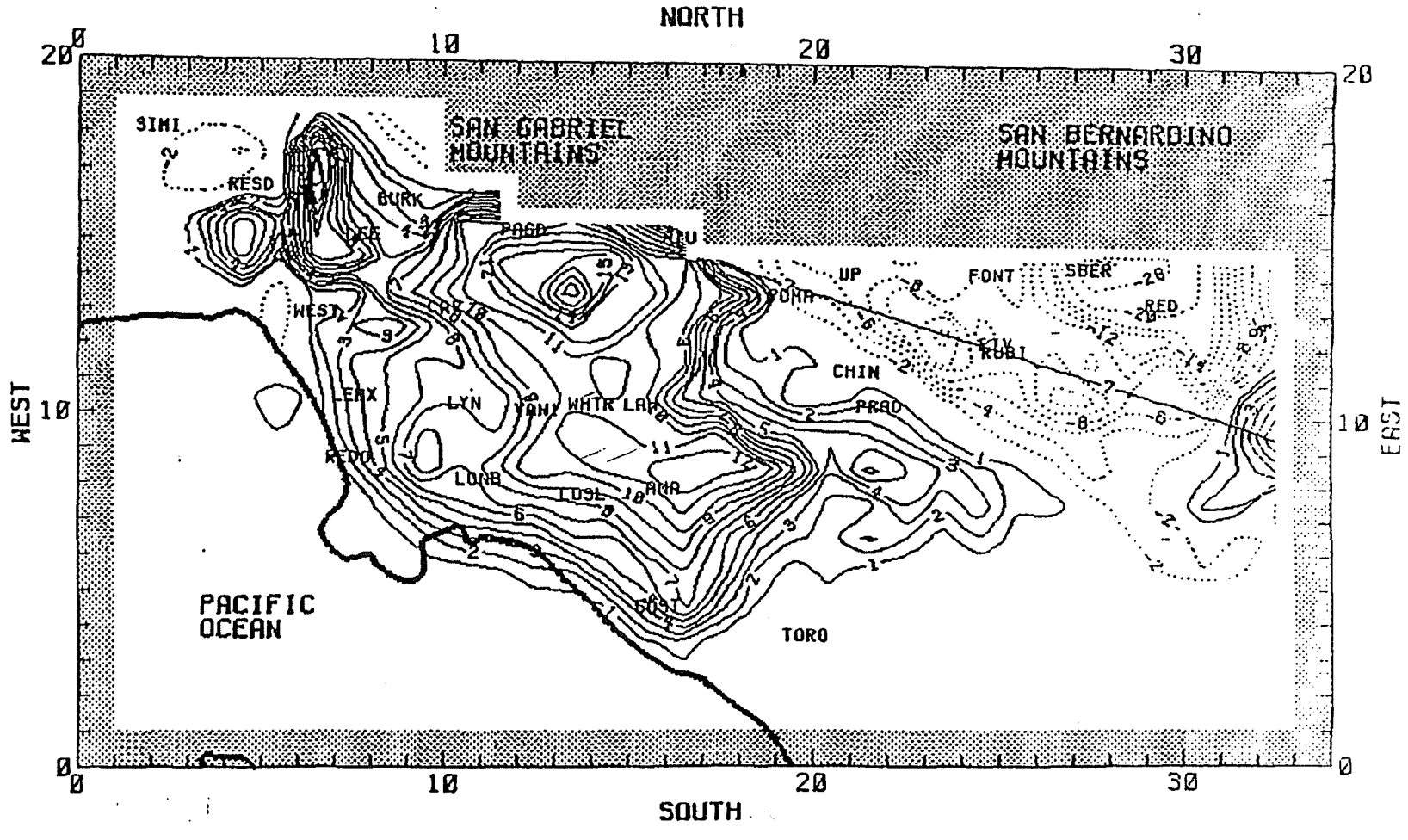


FIGURE III-7

PEAK OZONE CHANGES DUE TO EAST-WEST TRADEOFF (1.5:1) FOR NOx AND ROG
(CASE S5 - CASE S1)

(1) Scenario S_2

With 100 tons/day ROG and 128 tons/day NOx shifting from the west to the east, the peak ozone concentrations in the coastal and central portions of the Basin would likely increase and those in the two inland counties would likely decrease. The maximum increases and decreases are both about 1.2 pphm.

(2) Scenario S_3

A one-to-one trade-off of 100 tons/day NOx emission increase in the east for 100 tons/day ROG emissions reduction in the west would reduce the ozone concentration significantly throughout the Basin, especially in areas with Basinwide peak ozone concentrations. The Basinwide peak ozone concentration would be reduced by 3.5 pphm. This scenario represents a one-to-one west-to-east one-way trade-off between ROG and NOx emissions. However, it does indicate that Basidwide total NOx emissions would be increased with this approach.

(3) Scenario S_4

A west-to-east shift of 100 tons/day of ROG alone would likely reduce ozone concentration throughout the Basin with the exception of the far eastern portion of the San Bernardino County. The Basinwide peak ozone concentration would be lowered by about 2.0 pphm.

(4) Scenario S_5

This scenario involves one unit of NOx emission reduction and one half unit of ROG emission reduction in the west in exchange for one unit of NOx emission increase in the east. This approach would cause no net increase in Basinwide total NOx emissions and would reduce the Basinwide total ROG emission. The modeling results indicate that this would cause deterioration of peak ozone concentrations in most areas of the Basin with the exception of the San Bernardino County where peak ozone concentration would be reduced by about 1 pphm.

(5) Impacts to Areas Further Inland

With the introduction of new emissions in the eastern portion of the Basin, the results of all these modeling runs (S_2, S_3, S_4 and S_5) suggest that the peak ozone concentration east of the modeling area (east of Redlands) would likely be increased. The spatial extent (distance downwind) of such increases cannot be determined at this time.

Table III-2 compares the Basinwide ozone exposure on the second day of the two-day simulation for the four east-west emission trade-off scenarios (S_2, S_3, S_4 and S_5). Exposure is the time period in which the resident population exposed to ambient concentrations greater than or equal to a specific threshold level times the ambient concentration times the population exposed. The 1985 projected Basin population gridded into 5 by 5 km grid cells was used in this analysis. The grid cell is the basic unit for matching population and

TABLE III-2
COMPARISON OF BASINWIDE OZONE EXPOSURE UNDER DIFFERENT SCENARIOS

Case ID*	BASINWIDE OZONE EXPOSURE RELATIVE TO BASE CASE (%)**		
	Above 12 pphm	Above 15 pphm	Above 20 pphm
S2	100.0	98.7	78.8
S3	74.2	51.0	7.8
S4	81.9	76.2	53.9
S5	102.5	99.9	94.0
S6	98.5	94.3	76.3

* See Figure III-1 for description of modeling scenarios
** Ozone exposure for base case during the modeling day are:
2.75×10^7 person-hours above 12 pphm
1.41×10^7 person-hours above 15 pphm
1.99×10^6 person-hours above 20 pphm

concentration estimates. The following equation mathematically describes the calculation of ozone exposure:

$$\text{Exposure} = \sum_{\text{hour}=1}^{24} P(x,y) \cdot C(x,y,\text{hour}) \cdot F[C(x,y,\text{hour})-K]$$

where: $P(x,y)$ = Population in Grid Cell (x,y)
K = Threshold Level
$C(x,y,\text{hour})$ = Concentration Prediction at Cell(x,y) During One Specific Hour
F = 0; if $C(x,y,\text{hour}) < K$
1; if $C(x,y,\text{hour}) > \text{or} = K$

Table III-2 lists exposure for three different ozone thresholds; 12, 15, and 20 pphm. The resulting data indicates Scenario S_3 would result in the largest reduction in exposure.

III.3 0.4 grams/mile Control Program

Figure III-8 displays the predicted changes of peak ozone concentrations with the implementation of the newly adopted 0.4 grams/mile mobile source control measure and 85 tons/day concurrent ROG reduction projected for the period before the implementation of this NOx control measure (ie, around 1994). The modeling results indicate that with the exception of south Los Angeles County and north Orange County where minor (up to 0.3 pphm) increases of peak ozone concentrations are predicted, most of the Basin would experience improvement of ozone air quality. The Basinwide peak ozone concentrations is expected to be reduced by about 1.0 pphm.

Both the emission changes and the predicted ozone impacts are consistent with the historical progress of concurrent ROG and NOx control which led to small deterioration of ozone air quality in the coastal/central areas and great ozone improvements can be made in eastern areas where ozone concentrations are the highest in the Basin.

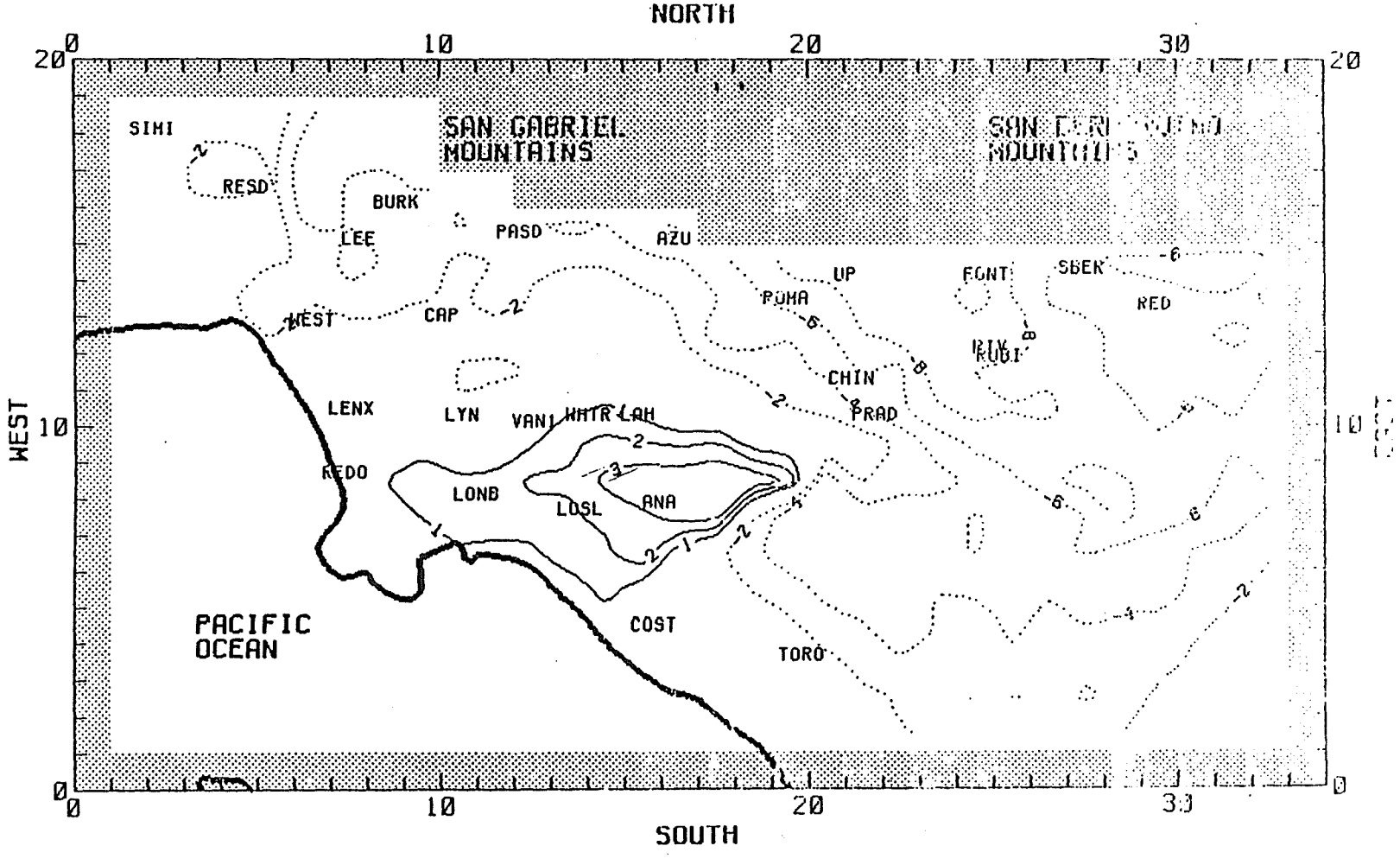


FIGURE III-8

PEAK OZONE CHANGES DUE TO 0.4 GRAM/MILE WITH CONCURRENT ROG CONTROL
(CASE S6 - CASE S1)

IV. CONCLUSIONS

IV.1 Treatment of Nighttime Chemistry

By not including the treatment of nighttime chemistry, previous UAM runs underestimated the peak ozone concentrations in the central position of the Basin and overpredicted the peak ozone concentrations in the inland areas. However, the magnitude of these differences are not significant enough to influence the policy implication derived from previous model runs.

IV.2 East-West Trade-Off

Aside from issues related to implementation feasibility, the most favorable trade-off approach (as far as ozone air quality is concerned) to accommodate growth of NOx emissions in the east portion of the Basin is to have equivalent reduction of ROG emissions in the western portion of the Basin. However, this approach would cause net increase in Basinwide total NOx emissions. A one-to-one East-West tradeoff for ROG emissions will generally cause Basinwide ozone reduction. A one-to-one west-to-east shift of NOx emissions and an equivalent west-to-east shift of both ROG and NOx emission are likely to cause deterioration of ozone air quality in the coastal and central portions of the Basin with some improvement in the eastern areas. An approach of having one-to-one west-to-east shift of NOx and additional small-scale ROG reduction in the western portion of the Basin would cause ozone to increase in large portion of the Basin.

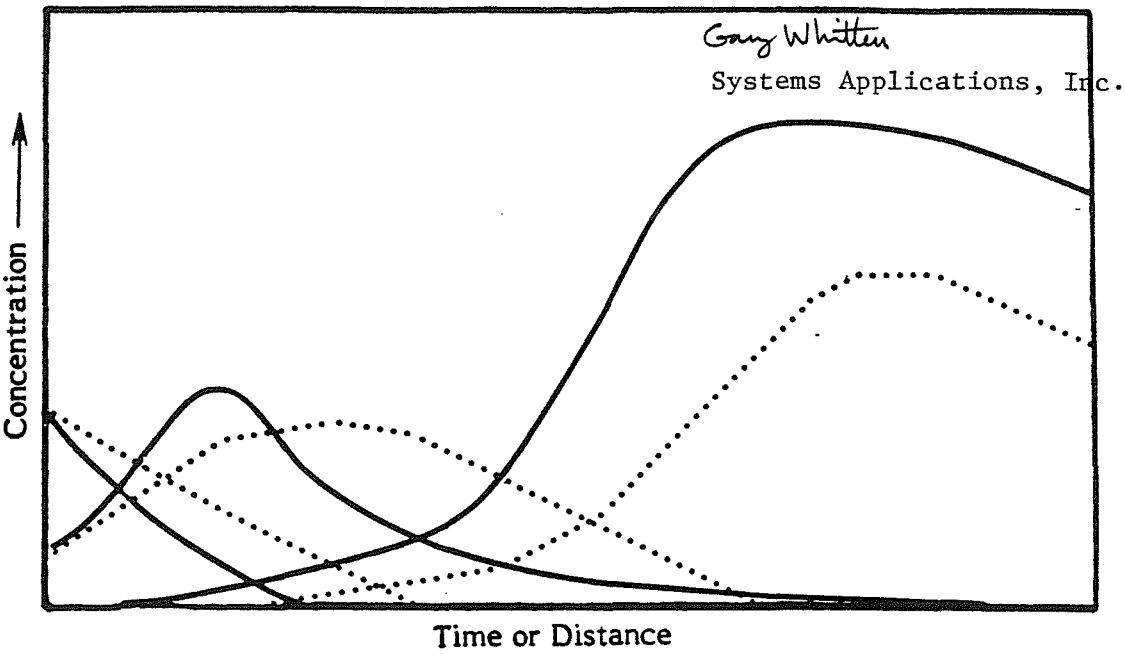
IV.3 0.4 grams/mile Control Program

The 0.4 grams/mile control with concurrent ROG emission reduction is a continuation of past practice of having concurrent controls on both ROG and NOx emissions. The model predicted future changes of ozone concentrations are consistent with historical experience: small increase in the coastal and central areas and great reduction in the inland area.

control

ROG

only

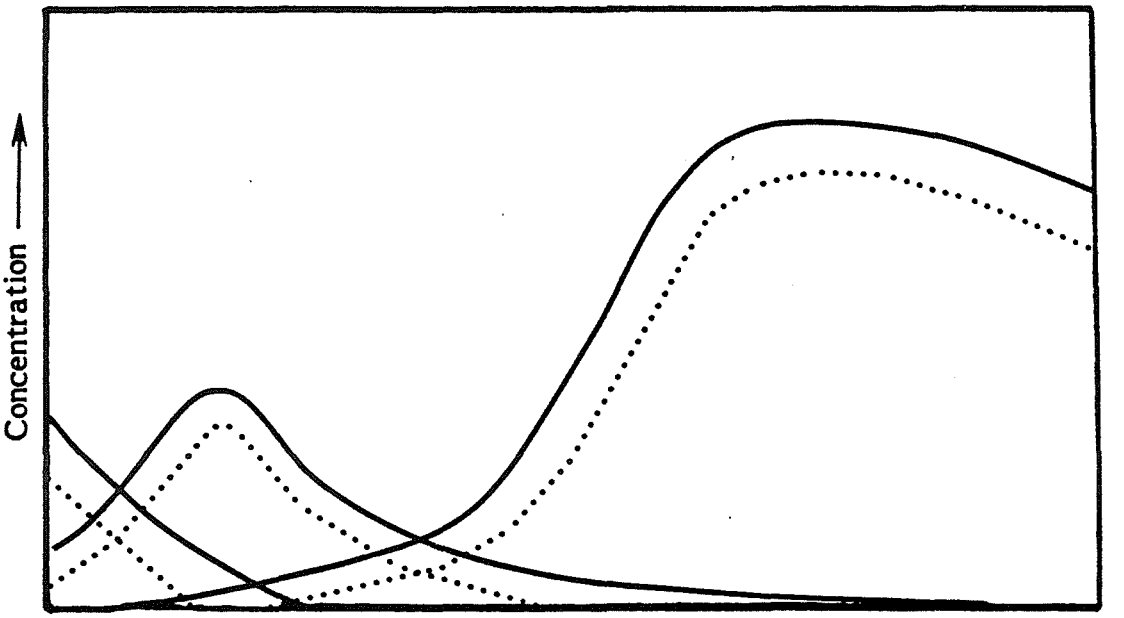


control

ROG

+

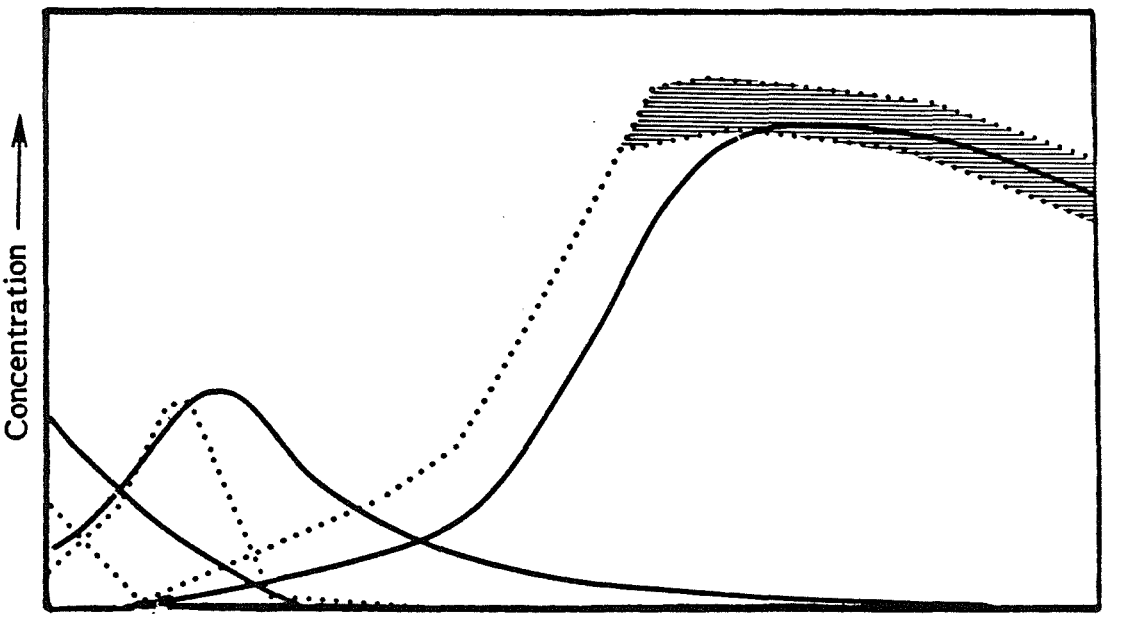
NO_X



control

NO_X

only



BASIC SMOG REACTIONS

$$O + O_2 \longrightarrow O_3$$

$$NO_2 + h\nu \longrightarrow O + NO$$

$$O_3 + NO \longrightarrow NO_2$$

$$HO_2^{\bullet} + NO \longrightarrow NO_2 + OH^{\bullet}$$

$$RO_2^{\bullet} + NO \longrightarrow NO_2 + RO^{\bullet}$$

ORGANIC CYCLE

$$OH^{\bullet} + VOC \longrightarrow RO_2^{\bullet} + H_2O \qquad k_{OH} = 3110$$

$$RO_2^{\bullet} + NO \longrightarrow NO_2 + RO^{\bullet}$$

$$RO^{\bullet} + O_2 \longrightarrow RCHO + HO_2$$

$$HO_2^{\bullet} + NO \longrightarrow NO_2 + OH^{\bullet}$$

RADICAL AND NO_2 SINK

$$OH^{\bullet} + NO_2 \longrightarrow HNO_3 \qquad k_{OH} = 17000$$

RADICAL SOURCES (PHOTOLYSIS)

$$RCHO^{\bullet} + hv \longrightarrow RO_2 + HO_2^{\bullet}$$

$$O_3 + hv \longrightarrow O_2 + O1D$$

$$O1D + H_2O \longrightarrow OH^{\bullet} + OH^{\bullet}$$

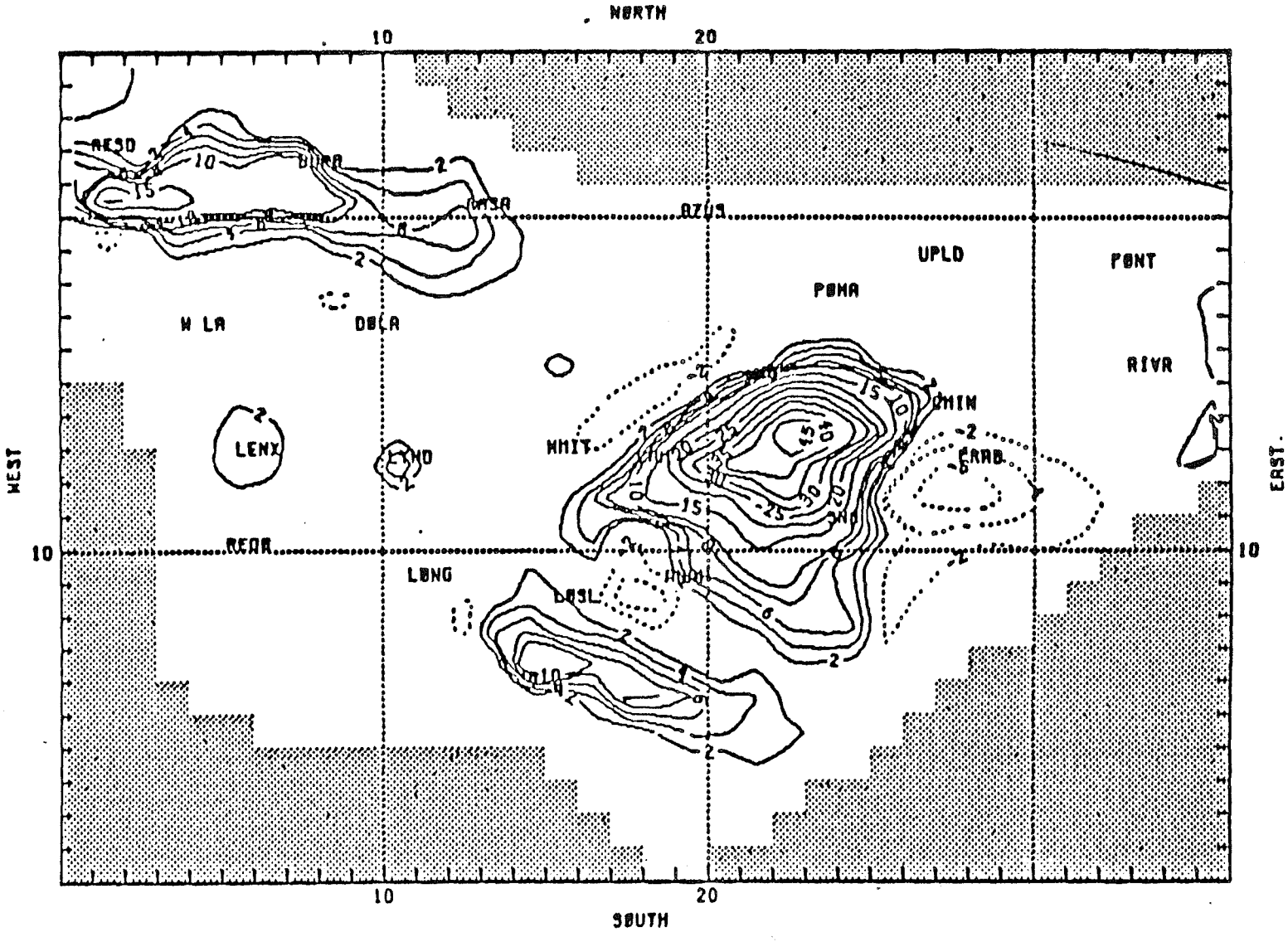
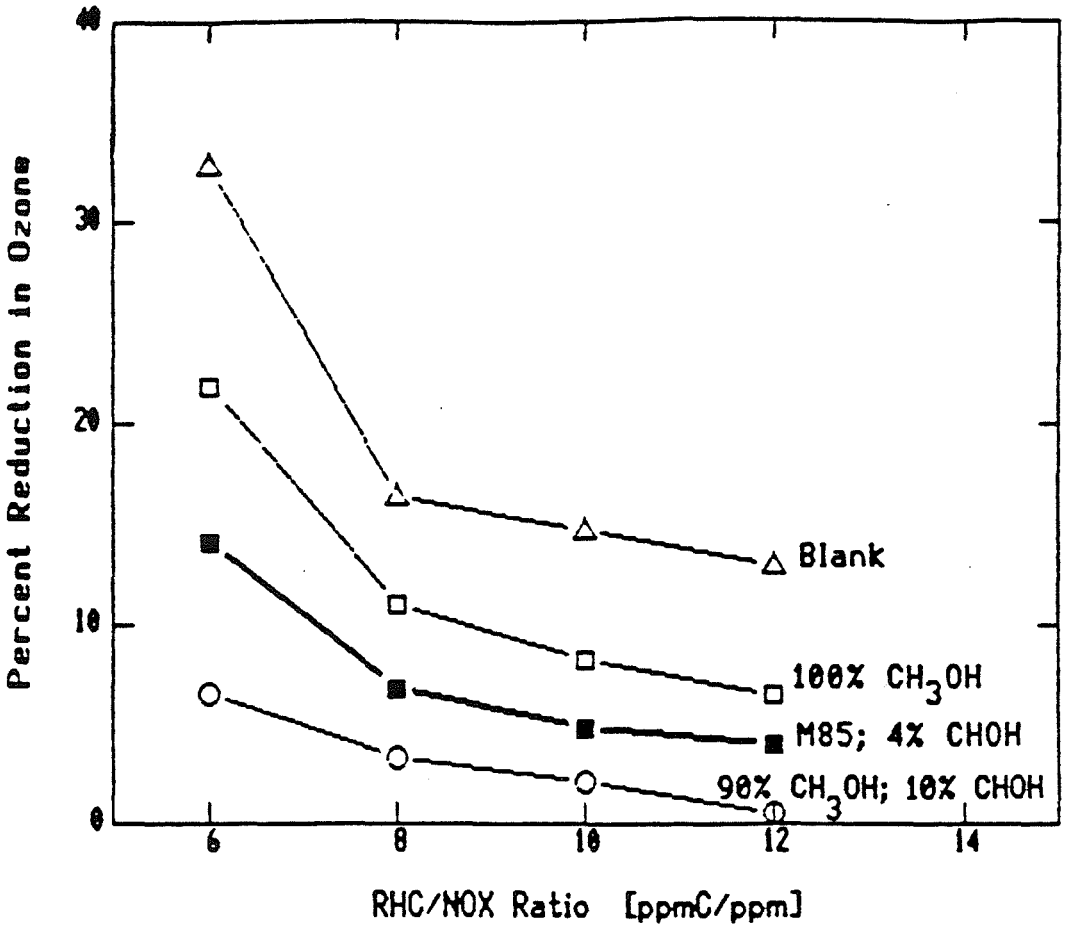


FIGURE DEFICIT-ENHANCEMENT PLOT OF THE HIGHEST ONE-HOUR NO_2 CONCENTRATIONS (ppb), SHOWING THE EFFECTS OF 90 PERCENT REDUCTION IN EMISSIONS



Source: R. J. Nichols and J. M. Norbeck (1985)

Fig. 1 Percentage reduction in ozone concentrations as a function of RHC/NOx ratio for different scenarios referred to in text. Dark line refers to scenario of 100% passenger car conversion to M85 fuel with 4% of total emissions formaldehyde.

ORGANIC CYCLE

$OH^{\bullet} + VOC \rightarrow RO_2^{\bullet} + H_2O$ $\quad k_{OH} = 3110$

$RO_2^{\bullet} + NO \rightarrow NO_2 + RO^{\bullet}$

$RO^{\bullet} + O_2 \rightarrow RCHO + HO_2$

$HO_2^{\bullet} + NO \rightarrow NO_2 + OH^{\bullet}$

RADICAL AND NO_2 SINK

$OH^{\bullet} + NO_2 \rightarrow HNO_3$ $\quad k_{OH} = 17000$

RADICAL SOURCES (PHOTOLYSIS)

$RCHO^{\bullet} + h\nu \rightarrow RO_2 + HO_2^{\bullet}$

$O_3 + h\nu \rightarrow O_2 + O1D$

$O1D + H_2O \rightarrow OH^{\bullet} + OH^{\bullet}$

HOW SHOULD REACTIVITY OF HYDROCARBON EMISSIONS BE CONSIDERED IN REGULATORY DECISIONS?

REGULATORY DECISIONS REGARDING HYDROCARBON (OR VOC) EMISSIONS SHOULD BE BASED ON CONSIDERATIONS OF ALL THEIR EFFECTS OF AIR QUALITY. OZONE FORMATION IS ONE OF THOSE EFFECTS.

VOC POLLUTANTS DIFFER IN THEIR EFFECTS ON OZONE FORMATION. THEIR EFFECTS ON OZONE IS MEASURED BY THEIR "REACTIVITIES"

CONSIDERATIONS OF VOC REACTIVITIES CAN BE USEFUL WHEN:

- THE MOST IMPORTANT AIR QUALITY IMPACT OF EMISSIONS OF THE VOC'S BEING CONSIDERED FOR CONTROL IS EFFECTS ON OZONE.
- VOC CONTROL HAS BEEN SHOWN TO BE AT LEAST AS BENEFICIAL TOWARDS REDUCING OZONE AS NO_x CONTROL
- THE REGULATIONS BEING CONSIDERED INCLUDE:
  - THOSE WHICH AFFECT EMISSIONS OF DIFFERENT TYPES OF VOC POLLUTANTS UNEQUALLY
  - THOSE WHICH INVOLVE SUBSTITUTION OF ONE TYPE OF VOC POLLUTANTS WITH OTHERS

EXAMPLES OF HOW REACTIVITY MIGHT BE PART OF A COST-BENEFIT ANALYSIS OF REGULATING EMISSIONS POLLUTANT "P" IN AN AIR BASIN

BENEFIT/COST OF REGULATING POLLUTANT "P"	=	BENEFIT OF REDUCING O_3 FORMED IN THE AIR BASIN	x	GRAMS O_3 FORMED PER GRAM "P" EMITTED IN THE AIR BASIN	÷	COST/TON OF REDUCING EMISSIONS OF POLLUTANT "P"

(REACTIVITY OF "P" UNDER CONDITIONS OF THE AIR BASIN)

EXAMPLE OF HOW REACTIVITY MIGHT BE PART OF AN ANALYSIS OF THE EFFECTS OF A VOC SUBSTITUTION STRATEGY

FOR A STRATEGY WHERE p_1 TONS OF POLLUTANT "P_1" WILL BE REPLACED BY p_2 TONS OF POLLUTANT "P_2"

$$\begin{array}{l}\text{TONS LESS OZONE} \\ \text{FORMED DUE TO} \\ \text{THE SUBSTITUTION} \\ \text{STRATEGY}\end{array} = p_1 \times \begin{array}{l}\text{GRAMS } O_3 \text{ FORMED} \\ \text{PER GRAM "}P_1\text{"} \\ \text{EMITTED}\end{array} - p_2 \times \begin{array}{l}\text{GRAMS } O_3 \text{ FORMED} \\ \text{PER GRAM "}P_2\text{"} \\ \text{EMITTED}\end{array}$$

$$\text{(REACTIVITY OF "}P_1\text{")} \qquad \text{(REACTIVITY OF "}P_2\text{")}$$

PROBLEMS IN DERIVING QUANTITATIVE, SCIENTIFICALLY JUSTIFIABLE REACTIVITY ESTIMATES FOR REGULATORY ASSESSMENT

1. THE REACTIVITY OF A COMPOUND CAN DEPEND SIGNIFICANTLY ON THE CONDITIONS OF THE AIRSHED INTO WHICH IT IS EMITTED:
   - HC/NO_x RATIO
   - AMOUNT AND REACTIVITIES OF OTHER VOC POLLUTANTS EMITTED ("BASE CASE" EMISSIONS)
   - WHERE AND WHEN EMITTED, DILUTION, TRANSPORT, METEOROLOGY, ETC. ("PHYSICAL SCENARIO")

2. REACTIVITY DEPENDS ON THE NATURE OF THE CHEMICAL:
   - HOW FAST IT REACTS IN THE ATMOSPHERE
   - HOW MUCH OZONE FORMATION (OR LOSS) IS CAUSED WHEN IT REACTS

3. EXISTING REACTIVITY CLASSIFICATION SCHEMES ARE QUALITATIVE AT BEST, AND DO NOT TAKE ALL THESE FACTORS INTO ACCOUNT.

REACTIVITIES ARE VERY DIFFICULT TO MEASURE DIRECTLY

- REACTION RATE MEASUREMENTS ALONE (USED TO DERIVE THE "OH REACTIVITY" SCALE) DO NOT MEASURE MECHANISTIC AND ENVIRONMENTAL EFFECTS ON REACTIVITY
- SMOG CHAMBER EXPERIMENTS WITH THE COMPOUND BY ITSELF DO NOT MEASURE INCREMENTAL REACTIVITIES IN POLLUTED ATMOSPHERES
- IT IS IMPRACTICAL FOR CHAMBER EXPERIMENTS TO REPRESENT THE RANGE OF CONDITIONS IN AIRSHEDS
- CHAMBER ARTIFACTS WILL ALWAYS AFFECT RESULTS OF CHAMBER EXPERIMENTS.

PROPOSED COMBINED EXPERIMENTAL AND MODELING APPROACH FOR ESTIMATING REACTIVITIES FOR REGULATORY PURPOSES:

1. DEVELOP AND TEST KINETIC MECHANISMS FOR ATMOSPHERIC REACTIONS OF MAJOR CURRENT VOC EMISSIONS. (SUCH MECHANISMS ARE ALREADY AVAILABLE)

2. DEVELOP AND TEST KINETIC MECHANISMS FOR COMPOUNDS WHOSE REACTIVITIES ARE OF INTEREST. (EXPERIMENTALLY TESTED MECHANISMS ARE AVAILABLE FOR SOME COMPOUNDS, NOT FOR MANY OTHERS)

3. DERIVE A SET OF MODEL SCENARIOS WHICH REPRESENT THE RANGE OF CONDITIONS OF THE AIRSHED(S) OF INTEREST. (WORK ON DEVELOPING INPUT TO EKMA MODELS CAN BE APPLIED TO THIS)

4. DO "BASE CASE" CALCULATIONS FOR THE REPRESENTATIVE SCENARIOS.

5. REPEAT "BASE CASE" CALCULATIONS WITH SMALL AMOUNT OF THE TEST COMPOUND ADDED TO THE VOC EMISSIONS ("TEST CALCULATIONS")

PROPOSED EXPERIMENTAL AND MODELING APPROACH FOR ESTIMATING REACTIVITIES FOR REGULATORY PURPOSES (CONTINUED):

6. DERIVE SETS OF REACTIVITIES FROM RESULTS OF "BASE CASE" AND "TEST" CALCULATIONS

$$\text{REACTIVITY} = \frac{\text{OZONE FORMED IN TEST CALCULATION} - \text{OZONE FORMED IN BASE CALCULATION}}{\text{AMOUNT OF TEST COMPOUND ADDED IN TEST CALCULATION}}$$

7. THE REACTIVITIES CALCULATED FOR THE SCENARIOS MOST REPRESENTATIVE OF OZONE POLLUTION EPISODES IN THE AIRSHED OF INTEREST CAN BE CONSIDERED IN CONTROL STRATEGY ANALYSES

ANALYSIS OF UNCERTAINTIES IN CALCULATED REACTIVITIES

REGULATORS NEED TO KNOW THE APPROXIMATE UNCERTAINTIES OF THESE REACTIVITY ESTIMATES

CALCULATIONS OF REACTIVITIES FOR CONTROL STRATEGY DEVELOPMENT SHOULD INCLUDE CALCULATIONS TO ASSESS HOW THE REACTIVITY ESTIMATES ARE AFFECTED BY:

1. THE RANGE OF METEOROLOGICAL CONDITIONS IN THE AIRSHED

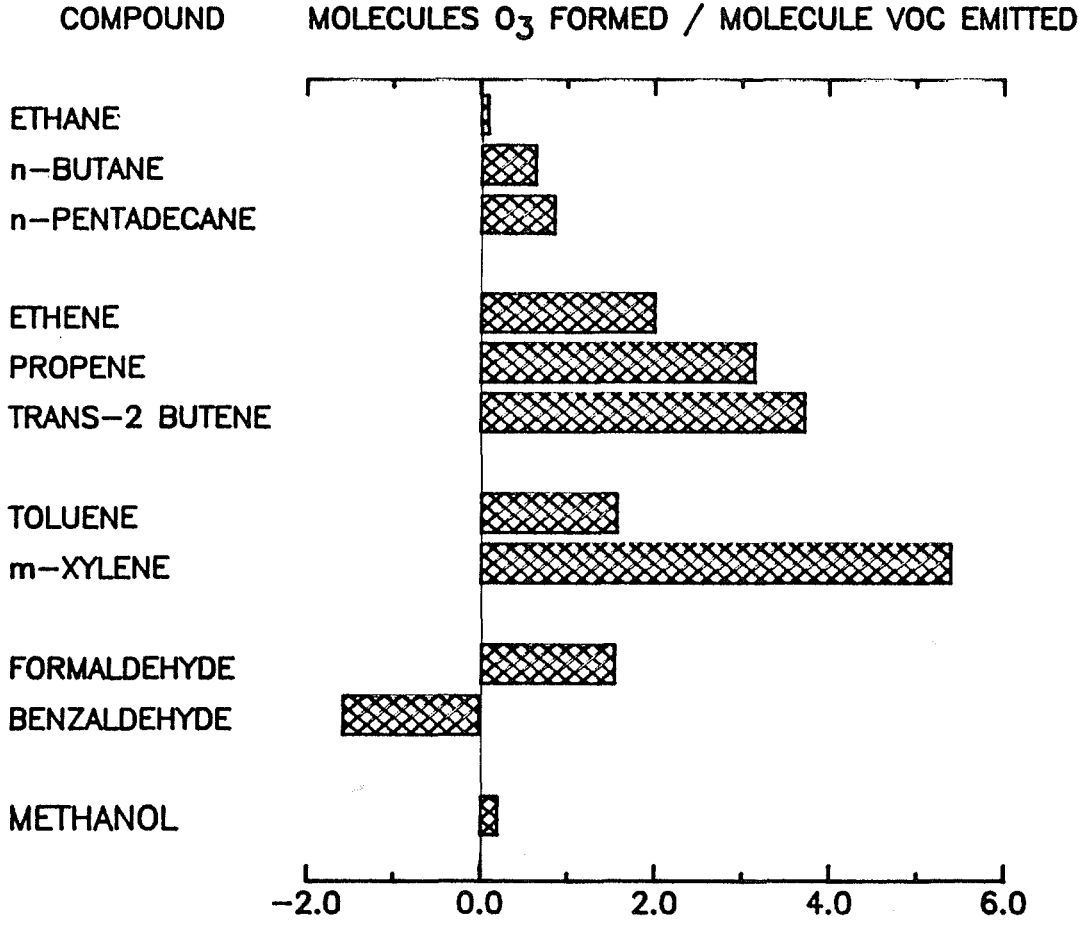
2. THE UNCERTAINTIES IN THE COMPOSITION OF THE CURRENT (BASE CASE) ROG EMISSIONS

3. THE UNCERTAINTIES IN THE ATMOSPHERIC CHEMISTRY OF THE TEST COMPOUND. (CALCULATIONS USING ALTERNATIVE MECHANISMS USEFUL HERE)

REACTIVITY CALCULATIONS USING SIMPLE (BOX OR TRAJECTORY) MODELS SHOULD BE CHECKED AGAINST SELECTED CALCULATIONS USING FULL AIRSHED MODELS

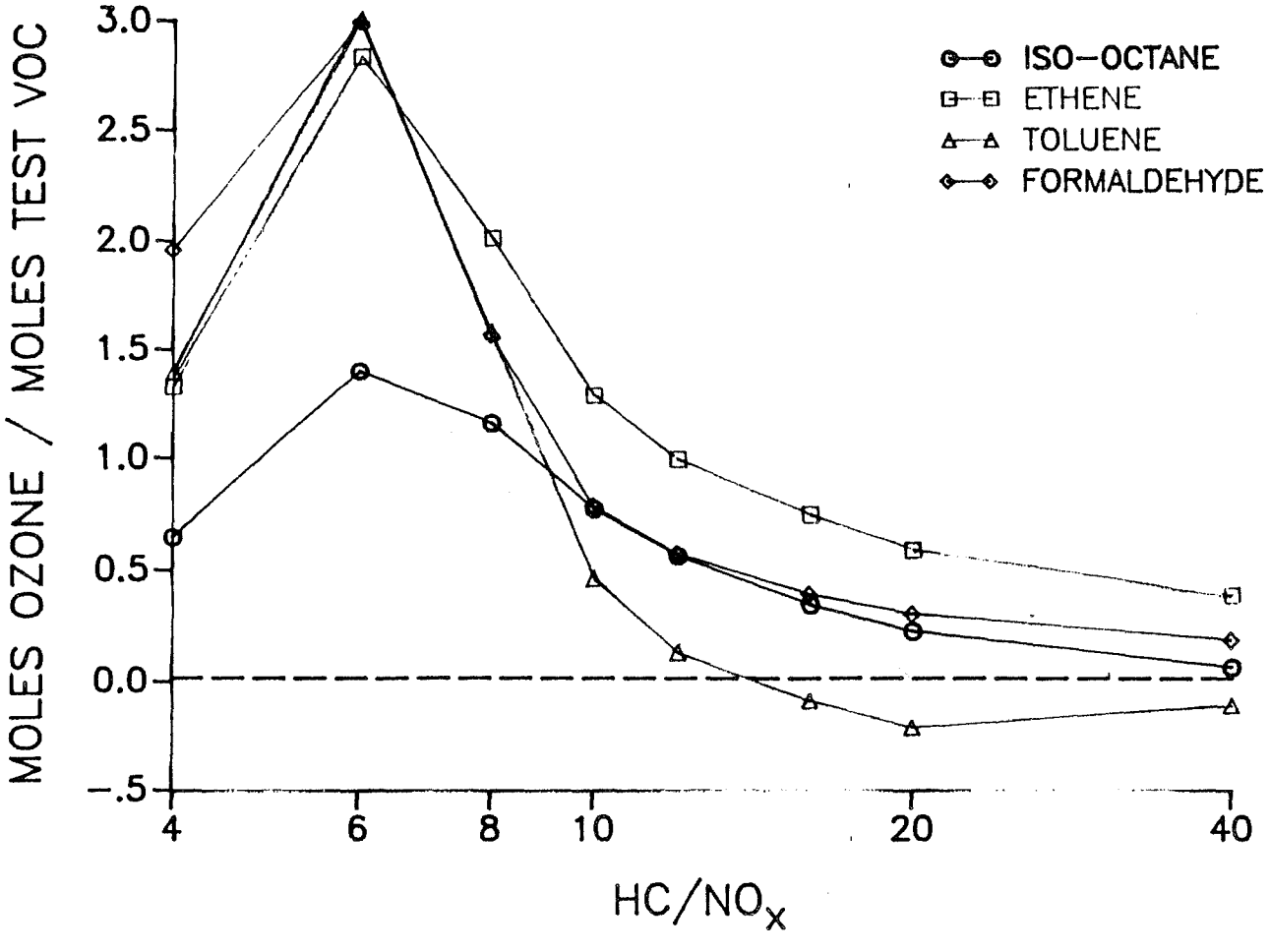
EXAMPLES OF CALCULATED REACTIVITIES FOR SELECTED COMPOUNDS
UNDER CONDITIONS FAVORABLE FOR OZONE FORMATION

PHYSICAL SCENARIO = EKMA DEFAULTS, "REGION 1" (LOW DILUTION)
ROG SURROGATE = EKMA DEFAULT
HC/NO_x RATIO = 8 ("OPTIMUM" FOR OZONE FORMATION)



DEPENDENCIES OF REACTIVITIES FOR SELECTED COMPOUNDS ON THE HC/NO_x RATIO

(EKMA, "REGION 1" SCENARIO, EKMA DEFAULT BASE CASE VOC)

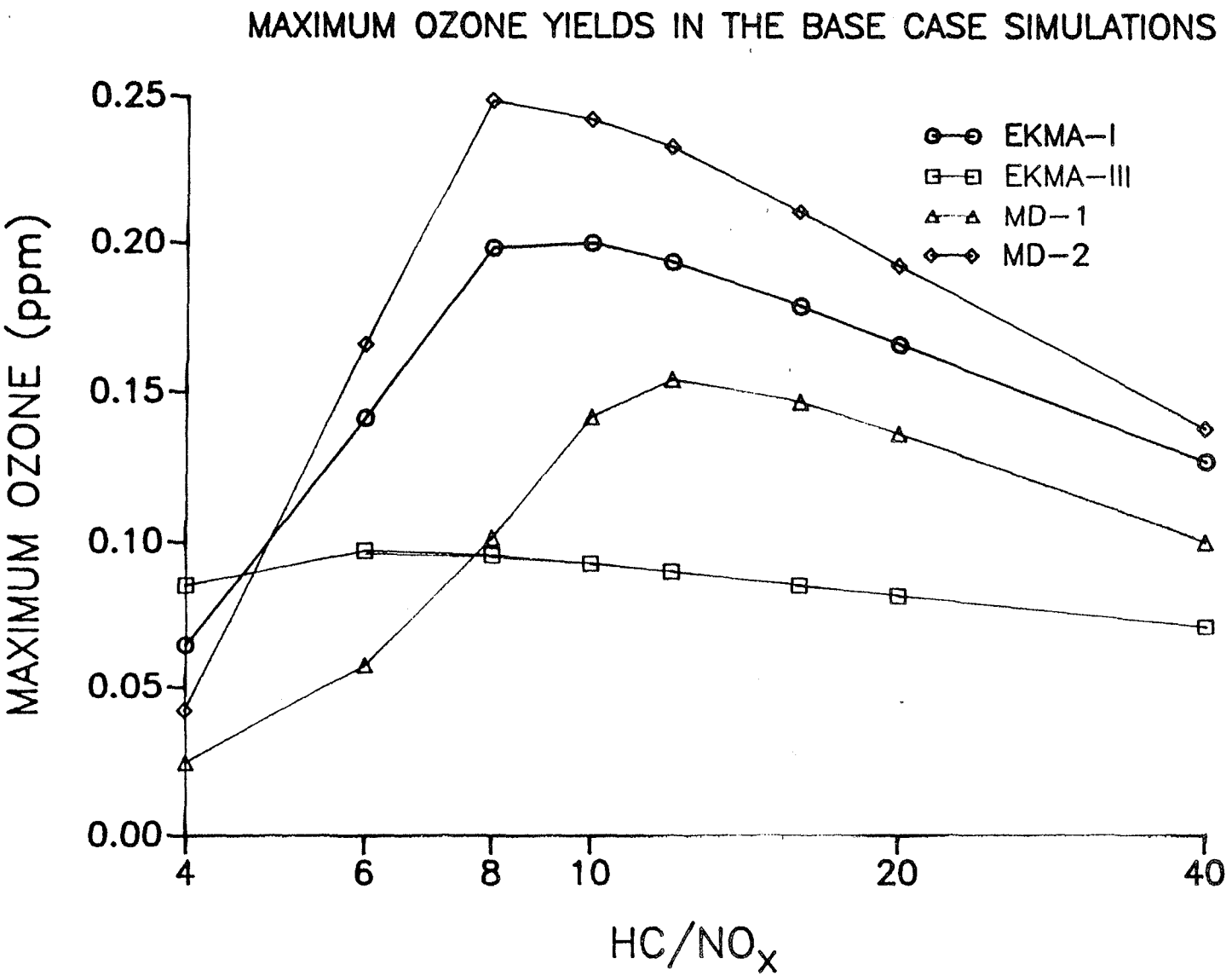


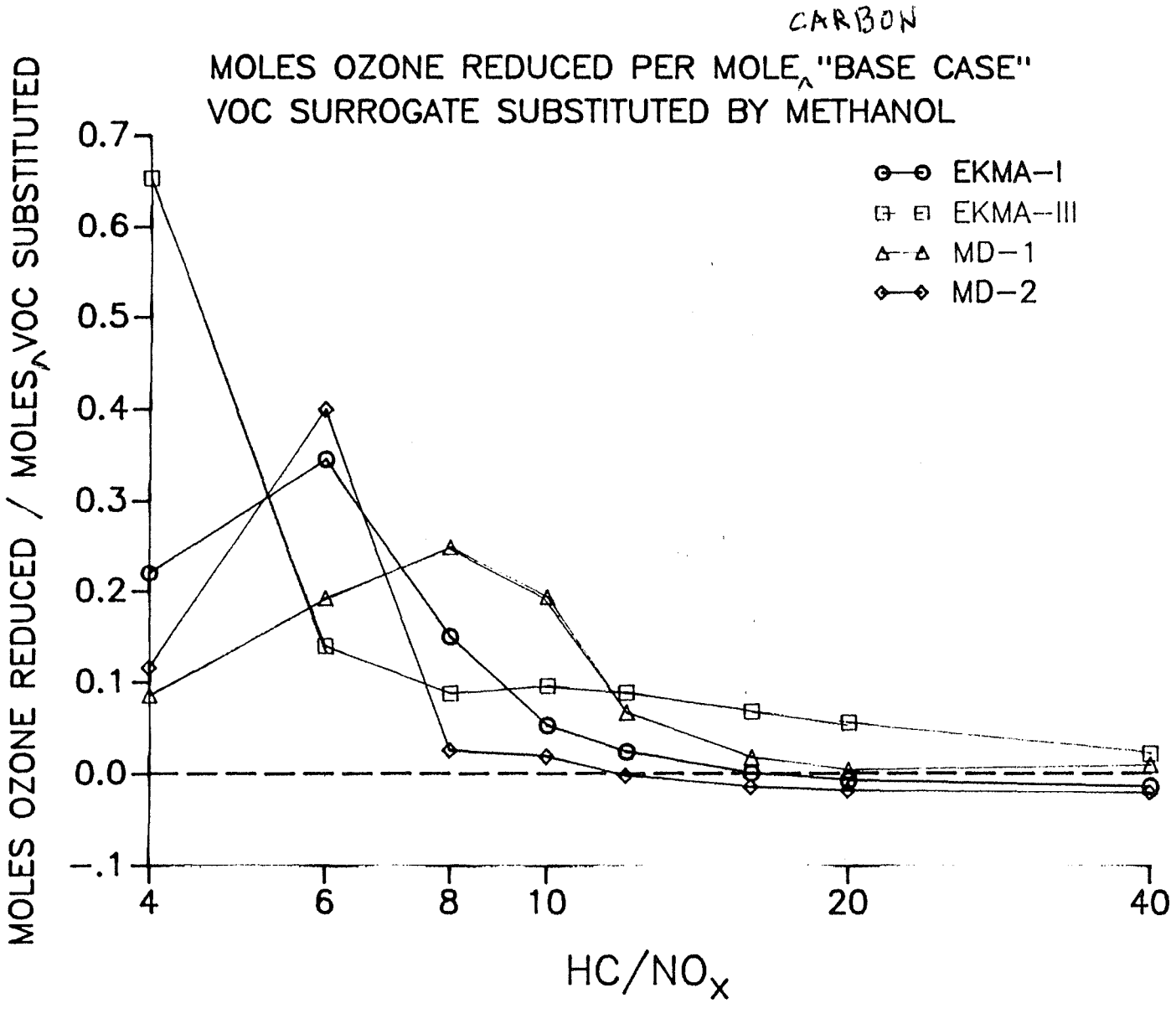
EXAMPLES OF APPLICATIONS OF CALCULATED REACTIVITIES

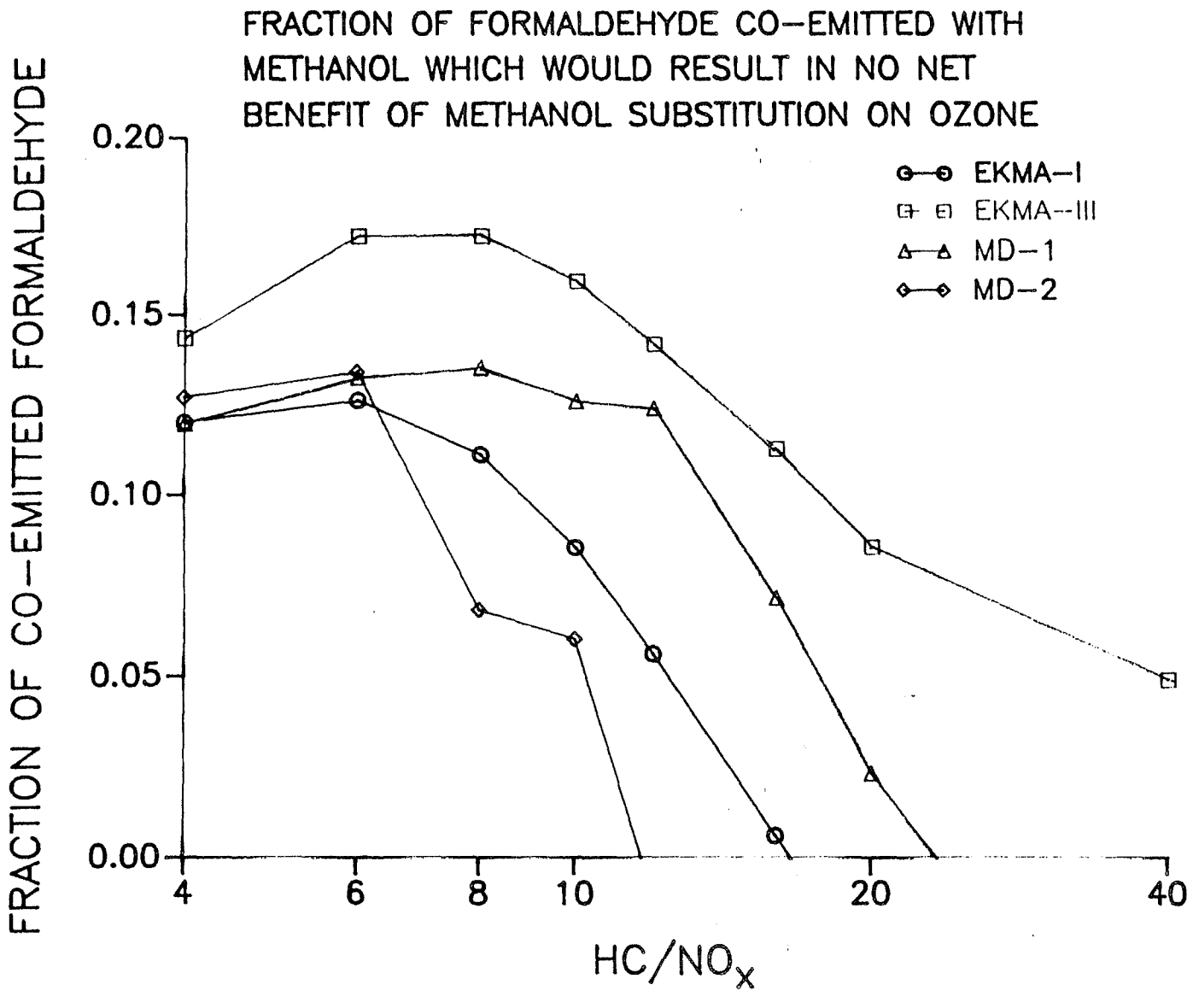
1. HOW WILL EFFECTS OF METHANOL SUBSTITUTION DEPEND ON CONDITIONS OF THE BASE CASE SCENARIO?

2. HOW MUCH FORMALDEHYDE CAN BE CO-EMITTED WITH METHANOL BEFORE NEGATING OZONE BENEFITS OF METHANOL SUBSTITUTION

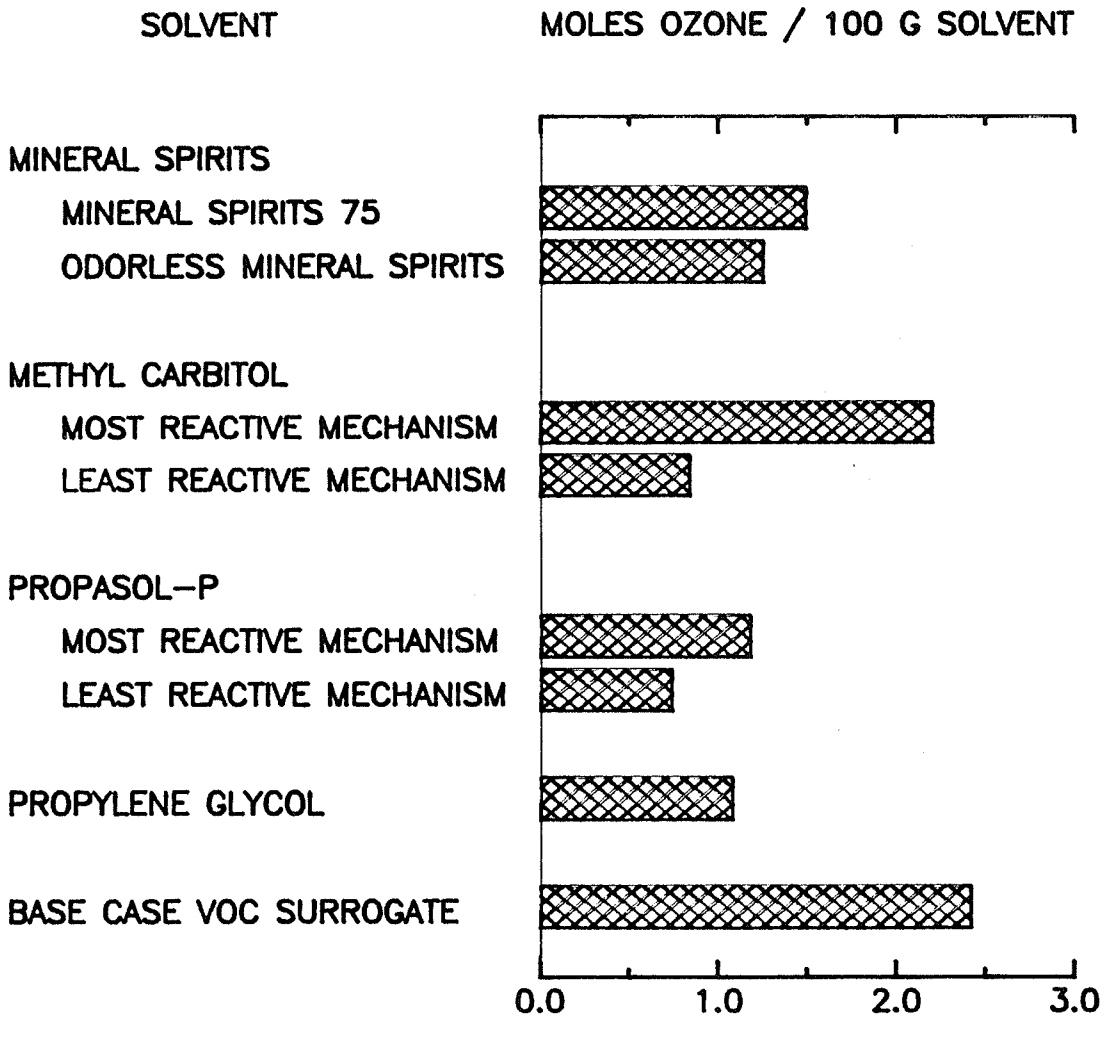
3. ARE SOLVENTS FOR WATER BASED PAINT SOLVENTS MUCH DIFFERENT IN REACTIVITY (PER GRAM) THAN THOSE FOR OIL BASED PAINTS?


MAXIMUM OZONE YIELDS IN THE BASE CASE SIMULATIONS
MAXIMUM OZONE (ppm)
0.25
0.20
0.15
0.10
0.05
0.00
4
6
8
10
20
40
HC/NOx
EKMA–I
EKMA–III
MD–1
MD–2


CARBON
MOLES OZONE REDUCED PER MOLE "BASE CASE" VOC SURROGATE SUBSTITUTED BY METHANOL
EKMA–I
EKMA–III
MD–1
MD–2
MOLES OZONE REDUCED / MOLES VOC SUBSTITUTED
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-.1
4
6
8
10
20
40
HC/NOx


FRACTION OF FORMALDEHYDE CO-EMITTED WITH METHANOL WHICH WOULD RESULT IN NO NET BENEFIT OF METHANOL SUBSTITUTION ON OZONE
EKMA-I
EKMA--III
MD-1
MD-2
FRACTION OF CO-EMITTED FORMALDEHYDE
0.20
0.15
0.10
0.05
0.00
4
6
8
10
20
40
HC/NOx

COMPARISON OF REACTIVITIES FOR SELECTED PAINT SOLVENTS
EKMA–1 SCENARIO, HC/NOX=8



CONCLUSIONS

A. ESTIMATION OF REACTIVITIES FOR REGULATORY ASSESSMENTS:

1. REACTIVITIES CANNOT PRESENTLY BE RELIABLY MEASURED BY DIRECT EXPERIMENT. USE OF MODEL CALCULATIONS IS UNAVOIDABLE

2. RELATIVELY INEXPENSIVE MODEL CALCULATIONS CAN BE USED TO MAKE REACTIVITY ESTIMATES WHICH TAKE MECHANISTIC AND ENVIRONMENTAL FACTORS INTO ACCOUNT

3. REACTIVITIES SHOULD BE CALCULATED FOR A WIDE RANGE OF CONDITIONS SO REGULATORS CAN ASSESS UNCERTAINTIES IN THE REACTIVITY ESTIMATES

4. FOR SCIENTIFICALLY JUSTIFIABLE REACTIVITY ESTIMATES, THE MODELS MUST EMPLOY EXPERIMENTALLY TESTED CHEMICAL MECHANISMS.

5. NECESSARY EXPERIMENTAL DATA EXIST FOR TESTING MECHANISMS FOR SOME, BUT NOT ALL, COMPOUNDS OF POTENTIAL REGULATORY INTEREST

CONCLUSIONS

B. USE OF REACTIVITY ESTIMATES IN REGULATORY DECISIONS

1. A QUANTITATIVE KNOWLEDGE OF REACTIVITIES CAN ASSIST REGULATORS IN DETERMINING THE MOST COST-EFFECTIVE VOC CONTROL STRATEGY FOR REDUCING OZONE

2. REGULATORS SHOULD NOT THINK REACTIVITIES AS SIMPLE ORDERINGS OR SCALES. THEY DEPEND ON THE CONDITIONS OF THE AIRSHED

3. REACTIVITIES CAN BE VERY DIFFERENT UNDER LOW NO_x COMPARED TO HIGH NO_x CONDITIONS. BUT VOC CONTROL IS INEFFECTIVE IN REDUCING OZONE WHEN NO_x IS LOW

4. REGULATORS SHOULD CONSIDER THE UNCERTAINTIES AND VARIABILITIES IN THE REACTIVITY ESTIMATES WHEN THEY ARE USED IN REGULATORY ANALYSES

5. CRITERIA OTHER THAN OZONE FORMATION MUST BE INCLUDED IN THE FULL ANALYSIS OF VOC CONTROL STRATEGIES